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Volume

A1

Symmetry relations between space groups

Edited by
Hans Wondratschek
and Ulrich Müller

First edition

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INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

*Volume A*1

SYMMETRY RELATIONS BETWEEN SPACE GROUPS

Edited by

HANS WONDRATSCHEK AND ULRICH MÜLLER

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Dedicated to

PAUL NIGGLI AND CARL HERMANN

In 1919, Paul Niggli (1888–1953) published the first compilation of space groups in a form that has been the basis for all later space-group tables, in particular for the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), for *International Tables for X-ray Crystallography* Volume I (1952) and for *International Tables for Crystallography* Volume A (1983). The tables in his book *Geometrische Kristallographie des Diskontinuums* (1919) contained lists of the *Punktlagen*, now known as *Wyckoff positions*. He was a great universal geoscientist, his work covering all fields from crystallography to petrology.

Carl Hermann (1899–1963) published among his seminal works four famous articles in the series *Zur systematischen Strukturtheorie* I to IV in *Z. Kristallogr.* **68** (1928) and **69** (1929). The first article contained the background to the Hermann–Mauguin space-group symbolism. The last article was fundamental to the theory of subgroups of space groups and forms the basis of the maximal-subgroup tables in the present volume. In addition, he was the editor of the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and one of the founders of n-dimensional crystallography, $n > 3$.

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Acknowledgments

Work on Parts 1 and 2 of this volume was spread out over a long period of time and there have been a number of colleagues and friends who have helped us in the preparation of this book. We are particularly grateful to Professor Th. Hahn, RWTH Aachen, Germany, not only for providing the initial impetus for this work but also for his constant interest and support. His constructive proposals on the arrangement and layout of the tables of Part 2 improved the presentation of the data and his stimulating comments contributed considerably to the content and the organization of Part 1, particularly Chapter 1.2.

Chapter 1.1 contains a contribution by Professor Y. Billiet, Bourg-Blanc, France, concerning isomorphic subgroups.

Nearly all contributors to this volume, but particularly Professors J. Neubüser and W. Plesken, RWTH Aachen, Germany, and Professor M. I. Aroyo, Universidad del País Vasco, Bilbao, Spain, commented on Chapter 1.2, correcting the text and giving valuable advice. Section 1.2.7 was completely reworked after intensive discussions with Professor V. Janovec, University of Liberec, Czech Republic, making use of his generously offered expertise in the field of domains.

In the late 1960s and early 1970s, J. Neubüser and his team at RWTH Aachen, Germany, calculated the basic lattices of non-isomorphic subgroups by computer. The results now form part of the content of the tables of Chapters 2.2 and 2.3. The team provided a great deal of computer output which was used for the composition of earlier versions of the present tables and for their checking by hand. The typing and checking of the original tables was done with great care and patience by Mrs R. Henke and many other members of the Institut für Kristallographie, Universität Karlsruhe, Germany.

The graphs of Chapters 2.4 and 2.5 were drawn and checked by Professor W. E. Klee, Dr R. Cruse and numerous students and technicians at the Institut für Kristallographie, Universität Karlsruhe, Germany, around 1970. M. I. Aroyo recently rechecked the graphs and transformed the hand-drawn versions into computer graphics.

We are grateful to Dr L. L. Boyle, University of Kent, Canterbury, England, who read, commented on and improved all parts of the text, in particular the English. We thank Professors J. M. Perez-Mato and G. Madariaga, Universidad del País Vasco, Bilbao, Spain, for many helpful discussions on the content and the presentation of the data. M. I. Aroyo would like to note that most of his contribution to this volume was made during his previous appointment in the Faculty of Physics, University of Sofia, Bulgaria, and he is grateful to his former colleagues, especially Drs J. N. Kotzev and M. Mikhov, for their interest and encouragement during this time.

We are indebted to Dr G. Nolze, Bundesanstalt für Materialforschung, Berlin, Germany, for checking the data of Chapter 3.2 using his computer program *POWDER CELL*. We also thank Mrs S. Funke and Mrs H. Sippel, Universität Kassel, Germany, who rechecked a large part of the relations of the Wyckoff positions in this chapter.

Mrs S. E. Barnes, Dr N. J. Ashcroft and the rest of the staff of the International Union of Crystallography in Chester took care of the successful technical production of this volume. In particular, we wish to thank Dr Ashcroft for her tireless help in matters of English style and her guidance in shaping the volume to fit the style of the *International Tables* series.

We gratefully acknowledge the financial support received from various organizations which helped to make this volume possible: in the early stages of the project from the Deutsche Forschungsgemeinschaft, Germany, and more recently from the Alexander von Humboldt-Stiftung, Germany, the International Union for Crystallography, the Sofia University Research Fund, Bulgaria, and the Universidad del País Vasco, Bilbao, Spain.

Contents

PART 3. RELATIONS BETWEEN THE WYCKOFF POSITIONS

Foreword

BY THEO HAHN

Symmetry and periodicity are among the most fascinating and characteristic properties of crystals by which they are distinguished from other forms of matter. On the macroscopic level, this symmetry is expressed by point groups, whereas the periodicity is described by translation groups and lattices, and the full structural symmetry of crystals is governed by space groups.

The need for a rigorous treatment of space groups was recognized by crystallographers as early as 1935, when the first volume of the trilingual series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* appeared. It was followed in 1952 by Volume I of *International Tables for X-ray Crystallography* and in 1983 by Volume A of *International Tables for Crystallography* (fifth edition 2002). As the depth of experimental and theoretical studies of crystal structures and their properties increased, particularly with regard to comparative crystal chemistry, polymorphism and phase transitions, it became apparent that not only the space group of a given crystal but also its 'descent' and 'ascent', *i.e.* its sub- and supergroups, are of importance and have to be derived and listed.

This had already been done in a small way in the 1935 edition of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* with the brief inclusion of the *translationengleiche* subgroups of the space groups (see the first volume, pp. 82, 86 and 90). The 1952 edition of *International Tables for X-ray Crystallography* did not contain sub- and supergroups, but in the 1983 edition of *International Tables for Crystallography* the full range of *maximal subgroups* was included (see Volume A, pp. 35–38): *translationengleiche* (type I) and *klassengleiche* (type II), the latter subdivided into 'decentred' (IIa), 'enlarged unit cell' (IIb) and 'isomorphic' (IIc) subgroups. For types I and IIa, *all* subgroups were listed individually, whereas for IIb only the *subgroup types* and for IIc only the *subgroups of lowest index* were given.

All these data were presented in the form known in 1983, and this involved certain omissions and shortcomings in the presentation, *e.g.* no Wyckoff positions of the subgroups and no conjugacy relations were given. Meanwhile, both the theory of subgroups and its application have made considerable progress, and the present Volume A1 is intended to fill the gaps left in Volume A and present the 'complete story' of the sub- and supergroups of space groups in a comprehensive manner. In particular, *all* maximal subgroups of types I, IIa and IIb are listed individually with the appropriate transformation matrices and origin shifts, whereas for the infinitely many maximal subgroups of type IIc expressions are given which contain the complete characterization of all isomorphic subgroups for any given index.

In addition, the relations of the Wyckoff positions for each group–subgroup pair of space groups are listed for the first time in the tables of Part 3 of this volume.

Volume A1 is thus a companion to Volume A, and the editors of both volumes have cooperated closely on problems of symmetry for many years. I wish Volume A1 the same acceptance and success that Volume A has enjoyed.

Scope of this volume

By Mois I. Aroyo, Ulrich Müller and Hans Wondratschek

Group–subgroup relations between space groups, the subject of this volume, are an important tool in crystallographic, physical and chemical investigations. In addition to listing these relations, the corresponding relations between the Wyckoff positions of the group–subgroup pairs are also listed here.

The basis for these tables was laid by the pioneering papers of Carl Hermann in the late 1920s. Some subgroup data were made available in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), together with a graph displaying the symmetry relations between the crystallographic point groups.

Since then, the vast number of crystal structures determined and improvements in experimental physical methods have directed the interest of crystallographers, physicists and chemists to the problems of structure classification and of phase transitions. Methods of computational mathematics have been developed and applied to the problems of crystallographic group theory and group–subgroup relations.

When the new series *International Tables for Crystallography* began to appear in 1983, the subgroup data that were then available were included in Volume A. However, these data were incomplete and their description was only that which was available in the late 1970s. This is still the case in the present (fifth) edition of Volume A.

The subgroup data for the space groups are now complete and form the basis of this volume. After introductory chapters on group-theoretical aspects of space groups, group–subgroup relations between space groups and the underlying mathematical background, this volume provides the reader (in many cases for the first time) with:

(1) complete listings of all maximal non-isomorphic subgroups for each space group, not just by type but individually, including their general positions or their generators, their conjugacy relations and transformations to conventional settings;

(2) listings of the maximal isomorphic subgroups with index 2, 3 or 4 individually in the same way as for non-isomorphic subgroups;

(3) listings of all maximal isomorphic subgroups as members of infinite series, but with the same information as for non-isomorphic subgroups;

(4) data for non-isomorphic supergroups for all space groups (these are already in Volume A) such that the subgroup data may be reversed for problems that involve supergroups of space groups;

(5) two kinds of graphs for all space groups displaying their types of *translationengleiche* subgroups and their types of non-isomorphic *klassengleiche* subgroups;

(6) listings of the splittings of all Wyckoff positions for each space group if its symmetry is reduced to that of a subgroup. These data include the corresponding coordinate transformations such that the coordinates in the subgroup can be obtained easily from the coordinates in the original space group;

(7) examples explaining how the data in this volume can be used.

The subgroup data in this volume are indispensable for a thorough analysis of phase transitions that do not involve drastic structural changes: the group–subgroup relations indicate the possible symmetry breaks that can occur during a phase transition and they are essential for determining the symmetry of the driving mechanism and the related symmetry of the resulting phase. The group–subgroup graphs describing the symmetry breaks provide information on the possible symmetry modes taking part in the transition and allow a detailed analysis of domain structures and twins. The subgroup relations between the space groups also determine the possible symmetries of intermediate phases that may be involved in the transition pathway in reconstructive phase transitions.

The data in this volume are invaluable for the construction of graphs of group–subgroup relations which visualize in a compact manner the relations between different polymorphic modifications involved in phase transitions and which allow the comparison of crystal structures and their classification into crystal-structure types. Particularly transparent graphs are the family trees that relate crystal structures in the manner developed by Bärnighausen (1980) (also called Bärnighausen trees), which also take into account the relations of the Wyckoff positions of the crystal structures considered. Such family trees display the additional degrees of freedom for the structural parameters of the low-symmetry phases, the possibilities of adapting to different kinds of distortions by reduction of site symmetries and the chemical variations (atomic substitutions) allowed for atomic positions that have become symmetry-independent.

The data on supergroups of space groups are useful for the prediction of high-temperature phase transitions, including the search for new ferroelectric and/or ferroelastic materials, for the treatment of the problem of overlooked symmetry in structure determination and for the study of phase transitions in which a hypothetical parent phase plays an important role.

Computer production of Parts 2 and 3

By Preslav Konstantinov, Asen Kirov, Eli B. Kroumova, Mois I. Aroyo and Ulrich Müller

The text and tables of this volume were produced electronically using the LaTeX 2ε typesetting system (Lamport, 1994), which has the following advantages:

(1) correcting and modifying the text, the layout and the data is easy;
(2) correcting or updating all of the above for future editions of this volume should also be simple;
(3) the cost of production for this first edition and for later editions should be kept low.

At first, sample input files for generating the tables of Part 2 for a few space groups were written which contained LaTeX 2ε instructions for creating both the page layout and the subgroup information. However, these files turned out to be rather complex and difficult to write and to adapt. It proved practically impossible to make changes in the layout. In addition, it could be foreseen that there would be many different layouts for the different space groups. Therefore, this method was abandoned. Instead, a separate data file was created for every space group in each setting listed in the tables. These files contained only the information about the subgroups and supergroups, encoded using specially created LaTeX 2ε commands and macros. These macros were defined in a separate package file which essentially contained the algorithm for the layout. Keeping the formatting information separate from the content as much as possible allowed us to change the layout by redefining the macros without changing the data files. This was done several times during the production of the tables.

The data files are relatively simple and only a minimal knowledge of LaTeX 2ε is required to create and revise them should it be necessary later. A template file was used to facilitate the initial data entry by filling blank spaces and copying pieces of text in a text editor. It was also possible to write computer programs to extract the information from the data files directly. Such programs were used for checking the data in the files that were used to typeset the volume. The data prepared for Part 2 were later converted into a more convenient, machine-readable format so that they could be used in the database of the Bilbao crystallographic server at http://www.cryst.ehu.es/.

The final composition of all plane-group and space-group tables of maximal subgroups and minimal supergroups was done by a single computer job. References in the tables from one page to another were automatically computed. The run takes 1 to 2 minutes on a modern workstation. The result is a PostScript file which can be fed to most laser printers or other modern printing/typesetting equipment.

The resulting files were also used for the preparation of the fifth edition of *International Tables for Crystallography* Volume A (2002) (abbreviated as *IT* A). Sections of the data files of Part 2 of the present volume were transferred directly to the data files for Parts 6 and 7 of *IT* A to provide the subgroup and supergroup information listed there. The formatting macros were rewritten to achieve the layout used in *IT* A.

The different types of data in the LaTeX 2ε files were either keyed by hand or computer-generated. The preparation of the data files of Part 2 can be summarized as follows:

Headline, origin: hand-keyed.
Generators: hand-keyed.
General positions: created by a program from a set of generators. The algorithm uses the well known generating process for space groups based on their solvability property, *cf.* Section 8.3.5 of *IT* A.
Maximal subgroups: hand-keyed. The data for the subgroup generators (or general-position representatives for the cases of *translationengleiche* subgroups and *klassengleiche* subgroups with 'loss of centring translations'), for transformation matrices and for conjugacy relations between subgroups were checked by specially designed computer programs.
Minimal supergroups: created automatically from the data for maximal subgroups.

The electronic preparation of the subgroup tables and the text of Part 2 was carried out on various Unix- and Windows-based computers in Sofia, Bilbao, Stuttgart and Karlsruhe. The development of the computer programs and the layout macros in the package file was done in parallel by different members of the team. Th. Hahn (Aachen) contributed to the final arrangement of the data.

The tables of Part 3 have a different layout, and a style file of their own was created for their production. Again, separate data files were prepared for every space group, containing only the information concerning the subgroups. The macros of the style file were developed by U. Müller, who also hand-keyed all files over the course of seven years.

Most of the data of Part 2 were checked using computer programs developed by F. Gähler (*cf.* Chapter 1.4) and A. Kirov. The relations of the Wyckoff positions (Part 3) were checked by G. Nolze (Berlin) with the aid of his computer program *POWDER CELL* (Nolze, 1996). In addition, all relations were cross-checked with the program *WYCKSPLIT* by Kroumova *et al.* (1998), with the exception of the positions of high multiplicities of some cubic space groups with subgroup indices > 50, which could not be handled by the program.

List of symbols and abbreviations used in this volume

(1) *Points and point space*

P, Q, R	points
O	origin
A_n, $\mathbb{A}_n$, P_n	n-dimensional affine space
E_n, $\mathbb{E}_n$	n-dimensional Euclidean point space
x, y, z; or x_i	point coordinates
$\boldsymbol{x}$	column of point coordinates
$\tilde{X}$	image point
$\tilde{\boldsymbol{x}}$	column of coordinates of an image point
$\tilde{x}_i$	coordinates of an image point
$\boldsymbol{x}'$	column of coordinates in a new coordinate system (after basis transformation)
x'_i	coordinates in a new coordinate system

(2) *Vectors and vector space*

$\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$; or $\mathbf{a}_i$	basis vectors of the space	
$\mathbf{r}$, $\mathbf{x}$	vectors, position vectors	
$\mathbf{o}$	zero vector (all coefficients zero)	
a, b, c	lengths of basis vectors	lattice parameters
α, β, γ; or α_j	angles between basis vectors	
$\boldsymbol{r}$	column of vector coefficients	
r_i	vector coefficients	
$(\mathbf{a})^{\mathrm{T}}$	row of basis vectors	
$\mathbf{V}_n$	n-dimensional vector space	

(3) *Mappings and their matrices and columns*

$\boldsymbol{A}$, $\boldsymbol{W}$	(3×3) matrices
$\boldsymbol{A}^{\mathrm{T}}$	matrix $\boldsymbol{A}$ transposed
$\boldsymbol{I}$	(3×3) unit matrix
A_{ik}, W_{ik}	matrix coefficients
$(\boldsymbol{A}, \boldsymbol{a})$, $(\boldsymbol{W}, \boldsymbol{w})$	matrix–column pairs
$\mathbb{W}$	augmented matrix
$\mathbb{x}$, $\tilde{\mathbb{x}}$, $\mathbb{t}$	augmented columns
$\boldsymbol{P}$, $\mathbb{P}$	transformation matrices
A, I, W	mappings
$\boldsymbol{w}$	column of the translation part of a mapping
w_i	coefficients of the translation part of a mapping
$\boldsymbol{G}$, G_{ik}	fundamental matrix and its coefficients
$\det(\ldots)$	determinant of a matrix
$\mathrm{tr}(\ldots)$	trace of a matrix

(4) *Groups*

$\mathcal{G}$	group; space group
$\mathcal{R}$	space group (Chapter 1.5)
$\mathcal{H}, \mathcal{U}$	subgroups of $\mathcal{G}$
$\mathcal{M}$	maximal subgroup of $\mathcal{G}$ (Chapter 1.5)
$\mathcal{M}$	Hermann's group (Chapter 1.2)
$\mathcal{P}$, $\mathcal{S}$, $\mathcal{V}$, $\mathcal{Z}$	groups
$\mathcal{T}(\mathcal{G})$, $\mathcal{T}(\mathcal{R})$	group of all translations of $\mathcal{G}$, $\mathcal{R}$
$\mathcal{A}$	group of all affine mappings = affine group
$\mathcal{E}$	group of all isometries (motions) = Euclidean group
$\mathcal{F}$	factor group
$\mathcal{I}$	trivial group, consisting of the unit element e only
$\mathcal{N}$	normal subgroup
$\mathcal{O}$	group of all orthogonal mappings = orthogonal group
$\mathcal{N}_{\mathcal{G}}(\mathcal{H})$	normalizer of $\mathcal{H}$ in $\mathcal{G}$
$\mathcal{N}_{\mathcal{E}}(\mathcal{H})$	Euclidean normalizer of $\mathcal{H}$
$\mathcal{N}_{\mathcal{A}}(\mathcal{H})$	affine normalizer of $\mathcal{H}$
$\mathcal{P}_{\mathcal{G}}$, $\mathcal{P}_{\mathcal{H}}$	point groups of the space groups $\mathcal{G}$, $\mathcal{H}$
$\mathcal{S}_{\mathcal{G}}(X)$, $\mathcal{S}_{\mathcal{H}}(X)$	site-symmetry groups of point X in the space groups $\mathcal{G}$, $\mathcal{H}$
a, b, g, h, m, t	group elements
e	unit element
i or $[i]$	index of $\mathcal{H}$ in $\mathcal{G}$

(5) *Symbols used in the tables*

p	prime number
n, n'	arbitrary positive integer numbers
q, r, u, v, w	arbitrary integer numbers in the given range
$\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	basis vectors of the space group
$\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$	basis vectors of the subgroup or supergroup
x, y, z	site coordinates in the space group
$t(1,0,0)$, $t(0,1,0), \ldots$	generating translations

(6) *Abbreviations*

HM symbol	Hermann–Mauguin symbol
IT A	*International Tables for Crystallography* Volume A
PCA	parent-clamping approximation
k-subgroup	*klassengleiche* subgroup
t-subgroup	*translationengleiche* subgroup

1.1. Historical introduction

BY MOIS I. AROYO, ULRICH MÜLLER AND HANS WONDRATSCHEK

1.1.1. The fundamental laws of crystallography

The documentation concerning group-theoretical aspects of group–subgroup relations and the rising importance of these relations in three-dimensional crystallography is scattered widely in the literature. This short review, therefore, cannot be exhaustive and may even be unbalanced if the authors have missed essential sources. Not included here is the progress made in the general theory of crystallographic groups, *e.g.* in higher dimensions, which is connected with the names of the mathematicians and physicists Ascher, Brown, Janner, Janssen, Neubüser, Plesken, Zassenhaus and others. This volume A1 of *International Tables for Crystallography*, abbreviated *IT* A1, is concerned with objects belonging to the 'classical' theory of crystallographic groups.

For a long time, the objective of crystallography, as implied by the word itself, was the description of crystals which were found in nature or which grew from solutions of salts or from melts. Crystals often display more-or-less planar faces which are symmetrically equivalent or can be made so by parallel shifting of the faces along their normals such that they form a regular body. The existence of characteristic angles between crystal faces was observed by Niels Stensen in 1669. The importance of the shape of crystals and their regularity was supported by observations on the cleavage of crystals. It was in particular this regularity which attracted mineralogists, chemists, physicists and eventually mathematicians, and led to the establishment of the laws by which this regularity was governed. The *law of symmetry* and the *law of rational indices* were formulated by René Just Haüy around 1800. These studies were restricted to the shape of macroscopic crystals and their physical properties, because only these were accessible to measurements until the beginning of the twentieth century.

Later in the nineteenth century, interest turned to 'regular systems' of points, for which the arrangement of points around every point is the same. These were studied by Wiener (1863) and Sohncke (1879). For such sets, there are isometric mappings of any point onto any other point which are such that they map the whole set onto itself. The primary aim was the classification and listing of such regular systems, while the groups of isometries behind these systems were of secondary importance. These regular systems were at first the sets of crystal faces, of face normals of crystal faces and of directions in crystals which are equivalent with respect to the physical properties or the symmetry of the external shape of the crystal. The listing and the classification of these finite sets was based on the *law of rational indices* and resulted in the derivation of the 32 crystal classes of point groups by Moritz Ludwig Frankenheim in 1826, Johann Friedrich Christian Hessel in 1830 and Axel V. Gadolin in 1867, cited by Burckhardt (1988). The list of this classification contained crystal classes that had not been observed in any crystal and included group–subgroup relations implicitly.

Crystal cleavage led Haüy in 1784 to assume small parallelepipeds as building blocks of crystals. In 1824, Ludwig August Seeber explained certain physical properties of crystals by placing molecules at the vertices of the parallelepipeds. The concepts of unit cell and of translation symmetry were thus introduced implicitly.

The classification of the 14 underlying lattices of translations was completed by Auguste Bravais (1850). In the second half of the nineteenth century, interest turned to the derivation and classification of *infinite* regular systems of points or figures, in particular by Leonhard Sohncke and Evgraf Stepanovich Fedorov. Sohncke, Fedorov (1891), Arthur Schoenflies (1891) and later William Barlow (1894) turned to the investigation of the underlying groups, the *space groups* and *plane groups*. The derivation and classification of these groups were completed in the early 1890s. It was a plausible hypothesis that the structures of crystals were related to combinations of regular systems of atoms (Haag, 1887) and that the symmetry of a crystal structure should be a space group, but both conjectures were speculations at that time with no experimental proof. This also applies to the atom packings described by Sohncke and Barlow, such as a model of the NaCl structure (which they did not assign to any substance).

1.1.2. Symmetry and crystal-structure determination

In 1895, Wilhelm Röntgen, then at the University of Würzburg, discovered what he called X-rays. Medical applications emerged the following year, but it was 17 years later that Max von Laue suggested at a scientific discussion in Munich that a crystal should be able to act as a diffraction grating for X-rays. Two young physicists, Walther Friedrich and Paul Knipping, successfully performed the experiment in May 1912 with a crystal of copper sulfate. In von Laue's opinion, the experiment was so important that he later publicly donated one third of his 1914 Nobel prize to Friedrich and Knipping. The discovery immediately aroused the curiosity of father William Henry Bragg and son William Lawrence Bragg. The son's experiments in Cambridge, initially with NaCl and KCl, led to the development of the Bragg equation and to the first crystal-structure determinations of diamond and simple inorganic materials. Since then, the determination of crystal structures has been an ever-growing enterprise.

The diffraction of X-rays by crystals is partly determined by the space group and partly by the relative arrangement of the atoms, *i.e.* by the atomic coordinates and the lattice parameters. The presentations by Fedorov and Schoenflies of the 230 space groups were not yet appropriate for use in structure determinations with X-rays. The breakthrough came with the fundamental book of Paul Niggli (1919), who described the space groups geometrically by symmetry elements and point positions and provided the first tables of what are now called *Wyckoff positions*. Niggli emphasized the importance of the multiplicity and site symmetry of the positions and demonstrated with examples the meaning of the *reflection conditions*.

Niggli's book pointed the way. The publication of related tables by Ralph W. G. Wyckoff (1922) included diagrams of the unit cells with special positions and symmetry elements. Additional tables by Astbury & Yardley (1924) listed 'abnormal spacings' for the space groups, *i.e.* the reflection conditions. These tables made the concepts and the data of geometric crystallography widely available and were the basis for the series *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) (abbreviated as *IT* 35), *International Tables for X-ray Crystallography*, Vol. I (1952, 1965, 1969) (abbreviated as *IT* 52) and *International Tables for Crystallography*, Vol. A (1983 and subsequent editions 1987, 1992, 1995, 2002) (abbreviated as *IT* A).

Group–subgroup relations were used in the original derivation of the space groups and plane groups. However, in the first decades of crystal-structure determinations, the derivation of geometric data (atomic coordinates) was of prime importance and the group-theoretical information in the publications was small, although implicitly present. With the growing number of crystal structures determined, however, it became essential to understand the rules and laws of crystal chemistry, to classify the incomprehensible set of structures into crystal-structure types, to develop methods for ordering the structure types in a systematic way, to show relations among them and to find common underlying principles.

To this end, different approaches were presented over time. By 1926, the number of crystal structures was already large enough for Viktor Moritz Goldschmidt to formulate basic principles of packing of atoms and ions in inorganic solids (Goldschmidt, 1926). Shortly afterwards, Linus Pauling (1928, 1929) formulated his famous rules about ionic radii, valence bonds, coordination polyhedra and the joining of these polyhedra. Later, Wilhelm Biltz (1934) focused attention on the volume requirements of atoms. Many other important factors determining crystal structures, such as chemical bonding, molecular shape, valence-electron concentration, electronic band structures, crystal-orbital overlap populations and others, have been the subject of subsequent studies. Each one of these aspects can serve as an ordering principle in crystal chemistry, giving insights from a different point of view.

For the aspects mentioned above, symmetry considerations are only secondary tools or even unimportant, and group–subgroup relations hardly play a role. Although symmetry is indispensable for the description of a specific crystal structure, for a long time crystal symmetry and the group–subgroup relations involved did not attract much attention as possible tools for working out the relations between crystal structures. This has even been the case for most textbooks on solid-state chemistry and physics. The lack of symmetry considerations is almost a characteristic feature of many of these books. There is a reason for this astonishing fact: the necessary group-theoretical material only became available in a useful form in 1965, namely as a listing of the maximal subgroups of all space groups by Neubüser & Wondratschek. However, for another 18 years this material was only distributed among interested scientists before it was finally included in the 1983 edition of *IT* A. And yet, even in the 2002 edition, the listing of the subgroups in Volume A is incomplete. It is this present Volume A1 which now contains the complete listing.

1.1.3. Development of the theory of group–subgroup relations

The systematic survey of group–subgroup relations of space groups started with the fundamental publication by Carl Hermann (1929). This paper is the last in a series of four publications, dealing with

(I) a nomenclature of the space-group types, a predecessor of the Hermann–Mauguin nomenclature;
(II) a method for the derivation of the 230 space-group types which is related to the nomenclature in (I);
(III) the derivation of the 75 types of rod groups and the 80 types of layer groups; and
(IV) the subgroups of space groups.

In paper (IV), Hermann introduced two distinct kinds of subgroups. The *translationengleiche* subgroups of a space group $\mathcal{G}$ have retained all translations of $\mathcal{G}$ but belong to a crystal class of lower symmetry than the crystal class of $\mathcal{G}$ (Hermann used the term *zellengleiche* instead of *translationengleiche*, see the footnote on page 17). The *klassengleiche* subgroups are those which belong to the same crystal class as $\mathcal{G}$, but have lost translations compared with $\mathcal{G}$. General subgroups are those which have lost translations as well as crystal-class symmetry. Hermann proved the theorem, later called *Hermann's theorem*, that any general subgroup is a *klassengleiche* subgroup of a uniquely determined *translationengleiche* subgroup of $\mathcal{G}$. In particular, this implies that a *maximal* subgroup of $\mathcal{G}$ is either a *translationengleiche* subgroup or a *klassengleiche* subgroup of $\mathcal{G}$.

Because of the strong relation (*homomorphism*) between a space group $\mathcal{G}$ and its point group $\mathcal{P}_{\mathcal{G}}$, the set of *translationengleiche* subgroups of $\mathcal{G}$ is in a one-to-one correspondence with the set of subgroups of the point group $\mathcal{P}_{\mathcal{G}}$. The crystallographic point groups are groups of maximal order 48 with well known group–subgroup relations and with not more than 96 subgroups. Thus, the maximal *translationengleiche* subgroups of any space group $\mathcal{G}$ can be obtained easily by comparison with the subgroups of its point group $\mathcal{P}_{\mathcal{G}}$. The kind of derivation of the space-group types by H. Heesch (1930) also gives access to *translationengleiche* subgroups. In *IT* 35, the types of the *translationengleiche* subgroups were listed for each space group [for a list of corrections to these data, see Ascher *et al.* (1969)]. A graph of the group–subgroup relations between the crystallographic point groups can also be found in *IT* 35; the corresponding graphs for the space groups were published by Ascher (1968). In these lists and graphs the subgroups are given only by their types, not individually.

The group–subgroup relations between the space groups were first applied in Vol. 1 of *Strukturbericht* (1931). In this volume, a crystal structure is described by the coordinates of the atoms, but the space-group symmetry is stated not only for spherical particles but also for molecules or ions with lower symmetry. Such particles may reduce the site symmetry and with it the space-group symmetry to that of a subgroup. In addition, the symmetry reduction that occurs if the particles are combined into larger structural units is stated. The listing of these detailed data was discontinued both in the later volumes of *Strukturbericht* and in the series *Structure Reports*. Meanwhile, experience had shown that there is no point in assuming a lower symmetry of the crystal structure if the geometrical arrangement of the centres of the particles does not indicate it.

With time, not only the classification of the crystal structures but also a growing number of investigations of (continuous) phase transitions increased the demand for data on subgroups of space groups. Therefore, when the Executive Committee of the International Union of Crystallography decided to publish a new series of *International Tables for Crystallography*, an extension of the subgroup data was planned. Stimulated and strongly supported by the mathematician J. Neubüser, the systematic derivation of the subgroups of the plane groups and the space groups began. The listing was restricted to the maximal subgroups of each space group, because any subgroup of a space group can be obtained by a chain of maximal subgroups.

The derivation by Neubüser & Wondratschek started in 1965 with the *translationengleiche* subgroups of the space groups, because the complete set of these (maximally 96) subgroups could be calculated by computer. All *klassengleiche* subgroups of indices 2, 3, 4, 6, 8 and 9 were also obtained by computer. As the index of a maximal non-isomorphic subgroup of a space group is restricted to 2, 3 or 4, *all* maximal non-isomorphic subgroups of all space groups were contained in the computer outputs. First results and their application to relations between crystal structures are found in Neubüser & Wondratschek (1966). In the early tables, the subgroups were only listed by their types. For *International Tables*, an extended list of maximal non-isomorphic subgroups was prepared. For each space group the maximal *translationengleiche* subgroups and those maximal *klassengleiche* subgroups for which the reduction of the translations could be described as 'loss of centring translations' of a centred lattice are listed individually. For the other maximal *klassengleiche* subgroups, *i.e.* those for which the conventional unit cell of the subgroup is larger than that of the original space group, the description by type was retained, because the individual subgroups of this kind were not completely known in 1983. The deficiency of such a description becomes clear if one realizes that a listed subgroup type may represent 1, 2, 3, 4 or even 8 individual subgroups.

In the present Volume A1, *all* maximal non-isomorphic subgroups are listed individually, in Chapter 2.2 for the plane groups and in Chapters 2.3 and 3.2 for the space groups. In addition, graphs for the *translationengleiche* subgroups (Chapter 2.4) and for the *klassengleiche* subgroups (Chapter 2.5) supplement the tables. After several rounds of checking by hand and after comparison with other listings, *e.g.* those by H. Zimmermann (unpublished) or by Neubüser and Eick (unpublished), intensive computer checking of the hand-typed data was carried out by F. Gähler as described in Chapter 1.4.

The mathematician G. Nebe describes general viewpoints and new results in the theory of subgroups of space groups in Chapter 1.5.

The maximal *isomorphic* subgroups are a special subset of the maximal *klassengleiche* subgroups. Maximal isomorphic subgroups are treated separately because each space group $\mathcal{G}$ has an infinite number of maximal isomorphic subgroups and, in contrast to non-isomorphic subgroups, there is no limit for the index of a maximal isomorphic subgroup of $\mathcal{G}$.

An *isomorphic subgroup* of a space group seems to have first been described in a crystal–chemical relation when the crystal structure of Sb_2ZnO_6 (structure type of tapiolite, Ta_2FeO_6) was determined by Byström *et al.* (1941): 'If no distinction is drawn between zinc and antimony, this structure appears as three cassiterite-like units stacked end-on-end' (Wyckoff, 1965). The space group of Sb_2ZnO_6 is a maximal isomorphic subgroup of index 3 with $\mathbf{c}' = 3\mathbf{c}$ of the space group $P4_2/mnm$ (D_{4h}^{14}, No. 136) of cassiterite SnO_2 (rutile type).

The first systematic study attempting to enumerate all isomorphic subgroups (not just maximal ones) for each space-group type was by Billiet (1973). However, the listing was incomplete and, moreover, in the case of enantiomorphic pairs of space-group types, only those with the same space-group symbol (called *isosymbolic space groups*) were taken into account.

Sayari (1976) derived the conventional bases for all maximal isomorphic subgroups of all plane groups. The general laws of number theory which underlie these results for plane-group types $p4$, $p3$ and $p6$ and space-group types derived from point groups 4, $\overline{4}$, $4/m$, 3, $\overline{3}$, 6, $\overline{6}$ and $6/m$ were published by Müller & Brelle (1995). Bertaut & Billiet (1979) suggested a new analytical approach for the derivation of all isomorphic subgroups of space and plane groups.

Because of the infinite number of maximal isomorphic subgroups, only a few representatives of lowest index are listed in *IT* A with their lattice relations but without origin specification, *cf.* *IT* A (2002), Section 2.2.15.2. Part 13 of *IT* A (Billiet & Bertaut, 2002) is fully devoted to isomorphic subgroups, *cf.* also Billiet (1980) and Billiet & Sayari (1984).

In this volume, all maximal isomorphic subgroups are listed as members of infinite series, where each individual subgroup is specified by its index, its generators and the coordinates of its conventional origin as parameters.

The relations between a space group and its subgroups become more transparent if they are considered in connection with their normalizers in the affine group $\mathcal{A}$ and the Euclidean group $\mathcal{E}$ (Koch, 1984). Even the corresponding normalizers of Hermann's group $\mathcal{M}$ play a role in these relations, *cf.* Wondratschek & Aroyo (2001).

In addition to subgroup data, supergroup data are listed in *IT* A. If $\mathcal{H}$ is a maximal subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a minimal supergroup of $\mathcal{H}$. In *IT* A, the type of a space group $\mathcal{G}$ is listed as a minimal non-isomorphic supergroup of $\mathcal{H}$ if $\mathcal{H}$ is listed as a maximal non-isomorphic subgroup of $\mathcal{G}$. Thus, for each space group $\mathcal{H}$ one can find in the tables the types of those groups $\mathcal{G}$ for which $\mathcal{H}$ is listed as a maximal subgroup. The supergroup data of *IT* A1 are similarly only an inversion of the subgroup data.

1.1.4. Applications of group–subgroup relations

Phase transitions. In 1937, Landau introduced the idea of the *order parameter* for the description of *second-order phase transitions* (Landau, 1937). Landau theory has turned out to be very useful in the understanding of phase transitions and related phenomena. Such a transition can only occur if there is a group–subgroup relation between the space groups of the two crystal structures. Often only the space group of one phase is known (usually the high-temperature phase) and subgroup relations help to eliminate many groups as candidates for the unknown space group of the other phase. Landau & Lifshitz (1980) examined the importance of group–subgroup relations further and formulated two theorems regarding the index of the group–subgroup pair. The significance of the subgroup data in second-order phase transitions was also pointed out by Ascher (1966, 1967), who formulated the *maximal-subgroup rule*: 'The symmetry group of a phase that arises in a ferroelectric transition is a maximal polar subgroup of the group of the high-temperature phase.' There are analogous applications of the maximal-subgroup rule (with appropriate modifications) to other types of continuous transitions.

The group-theoretical aspects of Landau theory have been worked out in great detail with major contributions by Birman (1966*a*,*b*), Cracknell (1975), Stokes & Hatch (1988), Tolédano & Tolédano (1987) and many others. For example, Landau theory gives additional criteria based on thermodynamic arguments for second-order phase transitions. The general statements are reformulated into group-theoretical rules which permit a phase-transition analysis without the tedious algebraic treatment involving high-order polynomials. The necessity of having complete subgroup data for the space groups for the successful implementation of these rules was stated by Deonarine & Birman (1983): '... there is a need for tables yielding for each of the 230 three-dimensional space groups a complete lattice of decomposition of all its subgroups.' Domain-structure analysis (Janovec & Přívratská, 2003) and symmetry-mode analysis (Aroyo & Perez-Mato, 1998) are further aspects of phase-transition problems where group–subgroup relations between space groups play an essential role. Domain structures are also considered in Section 1.2.7.

In treating successive phase transitions within Landau theory, Levanyuk & Sannikov (1971) introduced the idea of a hypothetical parent phase whose symmetry group is a supergroup of the observed (initial) space group. Moreover, the detection of pseudosymmetries is necessary for the prediction of higher-temperature phase transitions, *cf.* Kroumova *et al.* (2002) and references therein.

In a reconstructive phase transition, there is no group–subgroup relation between the symmetries of the two structures. Nevertheless, it has been pointed out that the 'transition path' between the two structures may involve an intermediate unstable structure whose space group is a common subgroup of the space groups of the two phases (Sowa, 2001; Stokes & Hatch, 2002).

Overlooked symmetry. In recent times, the number of crystal-structure determinations with a wrongly assigned space group has been increasing (Baur & Kassner, 1992; Marsh *et al.*, 2002). Frequently, space groups with too low a symmetry have been chosen. In most cases, the correct space group is a supergroup of the space group that has been assigned. A criterion for the correct assignment of the space group is given by Fischer & Koch (1983). Computer packages for treating the problem can be made more efficient if the possible supergroups are known.

Twinning can also lead to a wrong space-group assignment if it is not recognized, as a twinned crystal can feign a higher or lower symmetry. The true space group of the correct structure is usually a supergroup or subgroup of the space group that has been assumed (Nespolo & Ferraris, 2004).

Relations between crystal structures. Working out relations between different crystal structures with the aid of crystallographic group–subgroup relations was systematically developed by Bärnighausen (1980). The work became more widely known through a number of courses taught in Germany and Italy from 1976 to 1996 (in 1984 as a satellite meeting to the Congress of the International Union of Crystallography). For a script of the 1992 course, see Chapuis (1992). The basic ideas can also be found in the textbook by Müller (1993).

According to Bärnighausen, a family tree of group–subgroup relations is set up. At the top of the tree is the space group of a simple, highly symmetrical structure, called the *aristotype* by Megaw (1973) or the *basic structure* by Buerger (1947, 1951). The space groups of structures resulting from distortions or atomic substitutions (the *hettotypes* or *derivative structures*) are subgroups of the space group of the aristotype. Apart from many smaller Bärnighausen trees, some trees that interrelate large numbers of crystal structures have been published, *cf.* Section 1.3.1. Such trees may even include structures as yet unknown, *i.e.* the symmetry relations can also serve to predict new structure types that are derived from the aristotype; in addition, the number of such structure types can be calculated for each space group of the tree (McLarnan, 1981*a*,*b*,*c*; Müller, 1992, 1998, 2003).

Setting up a Bärnighausen tree not only requires one to find the group–subgroup relations between the space groups involved. It also requires there to be an exact correspondence between the atomic positions of the crystal structures considered. For a given structure, each atomic position belongs to a certain Wyckoff position of the space group. Upon transition to a subgroup, the Wyckoff position will or will not split into different Wyckoff positions of the subgroup. With the growing number of applications of group–subgroup relations there had been an increasing demand for a list of the relations of the Wyckoff positions for every group–subgroup pair. These listings are accordingly presented in Part 3 of this volume.

references

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1.2. General introduction to the subgroups of space groups

BY HANS WONDRATSCHEK

1.2.1. General remarks

The performance of simple vector and matrix calculations, as well as elementary operations with groups, are nowadays common practice in crystallography, especially since computers and suitable programs have become widely available. The authors of this volume therefore assume that the reader has at least some practical experience with matrices and groups and their crystallographic applications. The explanations and definitions of the basic terms of linear algebra and group theory in these first sections of this introduction are accordingly short. Rather than replace an elementary textbook, these first sections aim to acquaint the reader with the method of presentation and the terminology that the authors have chosen for the tables and graphs of this volume. The concepts of groups, their subgroups, isomorphism, coset decomposition and conjugacy are considered to be essential for the use of the tables and for their practical application to crystal structures; for a deeper understanding the concept of normalizers is also necessary. Frequently, however, an 'intuitive feeling' obtained by practical experience may replace a full comprehension of the mathematical meaning. From Section 1.2.6 onwards, the presentation will be more detailed because the subjects are more specialized (but mostly not more difficult) and are seldom found in textbooks.

1.2.2. Mappings and matrices

1.2.2.1. *Crystallographic symmetry operations*

A crystal is a finite block of an infinite periodic array of atoms in physical space. The infinite periodic array is called the *crystal pattern*. The finite block is called the *macroscopic crystal*.

Periodicity implies that there are *translations* which map the crystal pattern onto itself. Geometric mappings have the property that for each point P of the space, and thus of the object, there is a uniquely determined point $\tilde{P}$, the *image point*. The mapping is *reversible* if each image point $\tilde{P}$ is the image of one point P only.

Translations belong to a special category of mappings which leave all distances in the space invariant (and thus within an object and between objects in the space). Furthermore, a mapping of an object onto itself (German: *Deckoperation*) is the basis of the concept of geometric symmetry. This is expressed by the following two definitions.

Definition 1.2.2.1.1. A mapping is called a *motion*, a *rigid motion* or an *isometry* if it leaves all distances invariant (and thus all angles, as well as the size and shape of an object). In this volume the term 'isometry' is used. □

An isometry is a special kind of affine mapping. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but quotients of lengths on the same line are preserved. In Section 1.2.2.3, the description of affine mappings is discussed, because this type of description also applies to isometries. Affine mappings are important for the classification of crystallographic symmetries, *cf.* Section 1.2.5.2.

Definition 1.2.2.1.2. A mapping is called a *symmetry operation* of an object if

(1) it is an isometry,
(2) it maps the object onto itself. □

Instead of 'maps the object onto itself', one frequently says 'leaves the object invariant (as a whole)'. This does not mean that each point of the object is mapped onto itself; rather, the object is mapped in such a way that an observer cannot distinguish the states of the object before and after the mapping.

Definition 1.2.2.1.3. A symmetry operation of a crystal pattern is called a *crystallographic symmetry operation*. □

The symmetry operations of a macroscopic crystal are also crystallographic symmetry operations, but they belong to another kind of mapping which will be discussed in Section 1.2.5.4.

There are different types of isometries which may be crystallographic symmetry operations. These types are described and discussed in many textbooks of crystallography and in mathematical, physical and chemical textbooks. They are listed here without further treatment. Fixed points are very important for the characterization of isometries.

Definition 1.2.2.1.4. A point P is a *fixed point* of a mapping if it is mapped onto itself, *i.e.* the *image point* $\tilde{P}$ is the same as the original point P: $\tilde{P} = P$. □

The set of all fixed points of an isometry may be the whole space, a plane in the space, a straight line, a point, or the set may be empty (no fixed point).

The following kinds of isometries exist:

(1) The *identity operation*, which maps each point of the space onto itself. It is a symmetry operation of every object and, although trivial, is indispensable for the group properties which are discussed in Section 1.2.3.
(2) A *translation* t which shifts every object. A translation is characterized by its translation vector $\mathbf{t}$ and has no fixed point: if $\boldsymbol{x}$ is the column of coordinates of a point P, then the coordinates $\tilde{x}$ of the image point $\tilde{P}$ are $\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{t}$. If a translation is a symmetry operation of an object, the object extends infinitely in the directions of $\mathbf{t}$ and $-\mathbf{t}$. A translation preserves the 'handedness' of an object, *e.g.* it maps any right-hand glove onto a right-hand one and any left-hand glove onto a left-hand one.
(3) A *rotation* is an isometry that leaves one line fixed pointwise. This line is called the *rotation axis*. The degree of rotation about this axis is described by its rotation angle φ. In particular, a rotation is called an *N-fold rotation* if the rotation angle is $\varphi = k \times 360°/N$, where k and N are relatively prime integers. A rotation preserves the 'handedness' of any object.
(4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is now called the *screw axis*. The translation vector is called the *screw vector*. A screw rotation has no fixed points. The screw axis is invariant as a whole under the screw rotation but not pointwise.
(5) An N-fold *rotoinversion* is an N-fold rotation coupled with inversion through a point on the rotation axis. This point is called the *centre of the rotoinversion*. For $N \neq 2$ it is the only fixed point. The axis of the rotation is invariant as a whole

under the rotoinversion and is called its *rotoinversion axis*. A rotoinversion changes the handedness by its inversion component: it maps any right-hand glove onto a left-hand one and *vice versa*. Performed twice it results in a rotation. Special rotoinversions are those for $N = 1$ and $N = 2$, which are dealt with separately.

(6) The *inversion* can be considered as a onefold rotoinversion ($N = 1$). The fixed point is called the *inversion centre* or the *centre of symmetry*.

(7) A twofold rotoinversion ($N = 2$) is called a *reflection* or a *reflection through a plane*. It is an isometry which leaves a plane perpendicular to the twofold rotoinversion axis fixed pointwise. This plane is called the *reflection plane* or *mirror plane* and it intersects the rotation axis in the centre of the rotoinversion. Its orientation is described by the direction of its normal vector, *i.e.* of the rotation axis. For a twofold rotoinversion, neither the rotation nor the inversion are symmetry operations themselves. As for any other rotoinversion, the reflection changes the handedness of an object.

(8) A *glide reflection* is a reflection through a plane coupled with a translation parallel to this plane. The translation vector is called the *glide vector*. A glide reflection changes the handedness and has no fixed point. The former reflection plane is now called the *glide plane*. Under a glide reflection, the glide plane is invariant as a whole but not pointwise.

Symmetry operations of crystal patterns may belong to any of these isometries. The set of all symmetry operations of a crystal pattern has the following properties: performing two (and thus more) symmetry operations one after the other results in another symmetry operation. Moreover, there is the identity operation in this set, *i.e.* an operation that leaves every point of the space and thus of the crystal pattern fixed. Finally, for any symmetry operation of an object there is an 'inverse' symmetry operation by which its effect is reversed. These properties are necessary for the application of group theory, *cf.* Section 1.2.3.

1.2.2.2. *Coordinate systems and coordinates*

To describe mappings analytically, one introduces a coordinate system $\{O,\ \mathbf{a},\ \mathbf{b},\ \mathbf{c}\}$, consisting of three linearly independent (*i.e.* not coplanar) basis vectors $\mathbf{a},\ \mathbf{b},\ \mathbf{c}$ (or $\mathbf{a}_1,\ \mathbf{a}_2,\ \mathbf{a}_3$) and an origin O. For the plane (two-dimensional space) an origin and two linearly independent (*i.e.* not parallel) basis vectors $\mathbf{a},\ \mathbf{b}$ (or $\mathbf{a}_1,\ \mathbf{a}_2$) are chosen. Referred to this coordinate system, each point P can be described by three (or two for the plane) coordinates $x,\ y,\ z$ (or $x_1,\ x_2,\ x_3$). An object, *e.g.* a crystal, can now be described by a continuous or discontinuous function of the coordinates such as the electron density or the coordinates of the centres of the atoms. A mapping can be regarded as an instruction of how to calculate the coordinates $\tilde{x},\ \tilde{y},\ \tilde{z}$ of the image point $\tilde{X}$ from the coordinates $x,\ y,\ z$ of the original point X.

In contrast to the practice in physics and chemistry, a non-Cartesian coordinate system is usually chosen in crystallography. The primary aim of the choice of the crystallographic coordinate system is to describe the crystal pattern and its set of all symmetry operations in a simple way. This aim holds in particular for the infinitely many symmetry translations of the crystal pattern, which form its *translation group*. Secondary to this aim are equality of the lengths of, and right angles between, the basis vectors.

The vector $\mathbf{t}$ belonging to the translation t is called a *translation vector* or a *lattice vector*. The set of all translation vectors of the crystal pattern is called its *vector lattice* $\mathbf{L}$. Both the translation group and the vector lattice are useful tools for describing the periodicity of the crystals.

For the description of a vector lattice several kinds of bases are in use. Orthonormal bases are not the most convenient, because the coefficients of the lattice vectors may then be any real number. The coefficients of the lattice vectors are more transparent if the basis vectors themselves are lattice vectors.

Definition 1.2.2.2.1. A basis which consists of lattice vectors of a crystal pattern is called a *lattice basis* or a *crystallographic basis*. □

Referred to a lattice basis, each lattice vector $\mathbf{t} \in \mathbf{L}$ is a linear combination of the basis vectors with *rational coefficients*. One can even select special bases such that the coefficients of all lattice vectors are integers.

Definition 1.2.2.2.2. A crystallographic basis is called a *primitive basis* if *every* lattice vector has integer coefficients. □

A fundamental feature of vector lattices is that for any lattice in a dimension greater than one an infinite number of primitive bases exists. With certain rules, the choice of a primitive basis can be made unique (reduced bases). In practice, however, the *conventional bases* are not always primitive; the choice of a conventional basis is determined by the matrix parts of the symmetry operations, *cf.* Section 1.2.5.1.

1.2.2.3. *The description of mappings*

The instruction for the calculation of the coordinates of $\tilde{X}$ from the coordinates of X is simple for an affine mapping and thus for an isometry. The equations are

$$\begin{aligned}\tilde{x} &= W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1\\ \tilde{y} &= W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2\\ \tilde{z} &= W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3,\end{aligned} \qquad (1.2.2.1)$$

where the coefficients W_{ik} and w_j are constant. These equations can be written using the matrix formalism:

$$\begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix} = \begin{pmatrix}W_{11} & W_{12} & W_{13}\\ W_{21} & W_{22} & W_{23}\\ W_{31} & W_{32} & W_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} + \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix}. \qquad (1.2.2.2)$$

This matrix equation is usually abbreviated by

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}, \qquad (1.2.2.3)$$

where

$$\tilde{\boldsymbol{x}} = \begin{pmatrix}\tilde{x}\\ \tilde{y}\\ \tilde{z}\end{pmatrix},\ \boldsymbol{x} = \begin{pmatrix}x\\ y\\ z\end{pmatrix},\ \boldsymbol{w} = \begin{pmatrix}w_1\\ w_2\\ w_3\end{pmatrix} \text{ and } \boldsymbol{W} = \begin{pmatrix}W_{11} & W_{12} & W_{13}\\ W_{21} & W_{22} & W_{23}\\ W_{31} & W_{32} & W_{33}\end{pmatrix}.$$

Definition 1.2.2.3.1. The matrix $\boldsymbol{W}$ is called the *linear part* or *matrix part*, the column $\boldsymbol{w}$ is the *translation part* or *column part* of a mapping. □

In equations (1.2.2.1) and (1.2.2.3), the coordinates are mixed with the quantities describing the mapping, designated by the letters W_{ik} and w_j or $\boldsymbol{W}$ and $\boldsymbol{w}$. Therefore, one prefers to write equation (1.2.2.3) in the form

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W},\ \boldsymbol{w})\,\boldsymbol{x} \text{ or } \tilde{\boldsymbol{x}} = \{\boldsymbol{W}\,|\,\boldsymbol{w}\}\,\boldsymbol{x}. \qquad (1.2.2.4)$$

The symbols $(\boldsymbol{W},\ \boldsymbol{w})$ and $\{\boldsymbol{W}\,|\,\boldsymbol{w}\}$ which describe the mapping referred to the chosen coordinate system are called the *matrix–column pair* and the *Seitz symbol*.

The formulae for the combination of affine mappings and for the inverse of an affine mapping (regular matrix $\boldsymbol{W}$) are obtained by

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1 \boldsymbol{x} + \boldsymbol{w}_1, \; \tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2 \tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_3 \boldsymbol{x} + \boldsymbol{w}_3$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2 (\boldsymbol{W}_1 \boldsymbol{x} + \boldsymbol{w}_1) + \boldsymbol{w}_2 = \boldsymbol{W}_2 \boldsymbol{W}_1 \boldsymbol{x} + \boldsymbol{W}_2 \boldsymbol{w}_1 + \boldsymbol{w}_2.$$

From $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, it follows that $\boldsymbol{W}^{-1} \tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{W}^{-1} \boldsymbol{w}$ or $\boldsymbol{x} = \boldsymbol{W}^{-1} \tilde{\boldsymbol{x}} - \boldsymbol{W}^{-1} \boldsymbol{w}$.

Using matrix–column pairs, this reads

$$(\boldsymbol{W}_3, \boldsymbol{w}_3) = (\boldsymbol{W}_2, \boldsymbol{w}_2)(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1, \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2) \tag{1.2.2.5}$$

and

$$\boldsymbol{x} = (\boldsymbol{W}, \boldsymbol{w})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{W}', \boldsymbol{w}')\tilde{x}$$

or

$$(\boldsymbol{W}', \boldsymbol{w}') = (\boldsymbol{W}, \boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1}, -\boldsymbol{W}^{-1}\boldsymbol{w}). \tag{1.2.2.6}$$

One finds from equations (1.2.2.5) and (1.2.2.6) that the linear parts of the matrix–column pairs transform as one would expect:

(1) the linear part of the product of two matrix–column pairs is the product of the linear parts, *i.e.* if $(\boldsymbol{W}_3, \boldsymbol{w}_3) = (\boldsymbol{W}_2, \boldsymbol{w}_2)(\boldsymbol{W}_1, \boldsymbol{w}_1)$ then $\boldsymbol{W}_3 = \boldsymbol{W}_2 \boldsymbol{W}_1$;

(2) the linear part of the inverse of a matrix–column pair is the inverse of the linear part, *i.e.* if $(\boldsymbol{X}, \boldsymbol{x}) = (\boldsymbol{W}, \boldsymbol{w})^{-1}$, then $\boldsymbol{X} = \boldsymbol{W}^{-1}$. [This relation is included in the first one: from $(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{X}, \boldsymbol{x}) = (\boldsymbol{W}\boldsymbol{X}, \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{o})$ follows $\boldsymbol{X} = \boldsymbol{W}^{-1}$. Here $\boldsymbol{I}$ is the unit matrix and $\boldsymbol{o}$ is the column consisting of zeroes].

These relations will be used in Section 1.2.5.4.

For the column parts, equations (1.2.2.5) and (1.2.2.6) are less convenient:

$$(1)\; \boldsymbol{w}_3 = \boldsymbol{W}_2 \boldsymbol{w}_1 + \boldsymbol{w}_2; \qquad (2)\; \boldsymbol{w}' = -\boldsymbol{W}^{-1}\boldsymbol{w}.$$

Because of the inconvenience of these relations, it is often preferable to use 'augmented' matrices, by which one can describe the combination of affine mappings and the inverse mapping by the equations of the usual matrix multiplication. These matrices are introduced in the next section.

1.2.2.4. *Matrix–column pairs and $(n+1) \times (n+1)$ matrices*

It is natural to combine the matrix part and the column part describing an affine mapping to form a (3×4) matrix, but such matrices cannot be multiplied by the usual matrix multiplication and cannot be inverted. However, if one supplements the (3×4) matrix by a fourth row '0 0 0 1', one obtains a (4×4) square matrix which can be combined with the analogous matrices of other mappings and can be inverted. These matrices are called *augmented matrices* and are designated by open-face letters in this volume:

$$\mathbb{W} = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \quad \tilde{\mathbb{x}} = \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right), \quad \mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right). \tag{1.2.2.7}$$

In order to write equation (1.2.2.3) as $\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}$ with the augmented matrices $\mathbb{W}$, the columns $\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}$ also have to be extended to the augmented columns $\mathbb{x}$ and $\tilde{\mathbb{x}}$. Equations (1.2.2.5) and (1.2.2.6) then become

$$\mathbb{W}_3 = \mathbb{W}_2 \mathbb{W}_1 \text{ and } (\mathbb{W})^{-1} = (\mathbb{W}^{-1}). \tag{1.2.2.8}$$

The vertical and horizontal lines in the matrix have no mathematical meaning. They are simply a convenience for separating the matrix part from the column part and from the row '0 0 0 1', and could be omitted.

Augmented matrices are very useful when writing down general formulae which then become more transparent and more elegant. However, the matrix–column pair formalism is, in general, advantageous for practical calculations.

For the augmented columns of vector coefficients, see Section 1.2.2.6.

1.2.2.5. *Isometries*

Isometries are special affine mappings, as in Definition 1.2.2.1.1. The matrix $\boldsymbol{W}$ of an isometry has to fulfil conditions which depend on the coordinate basis. These conditions are:

(1) A basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ is characterized by the scalar products $(\mathbf{a}_j\, \mathbf{a}_k)$ of its basis vectors or by its *lattice parameters* a, b, c, α, β and γ. Here a, b, c are the lengths of the basis vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and α, β and γ are the angles between $\mathbf{a}_2$ and $\mathbf{a}_3$, $\mathbf{a}_3$ and $\mathbf{a}_1$, $\mathbf{a}_1$ and $\mathbf{a}_2$, respectively. The *metric matrix* $\boldsymbol{M}$ (called $\mathbf{G}$ in *IT* A, Chapter 9.1) is the (3×3) matrix which consists of the scalar products of the basis vectors:

$$\boldsymbol{M} = \begin{pmatrix} a^2 & a\,b\,\cos\gamma & a\,c\,\cos\beta \\ b\,a\,\cos\gamma & b^2 & b\,c\,\cos\alpha \\ c\,a\,\cos\beta & c\,b\,\cos\alpha & c^2 \end{pmatrix}.$$

If $\boldsymbol{W}$ is the matrix part of an isometry, referred to the basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$, then $\boldsymbol{W}$ must fulfil the condition $\boldsymbol{W}^{\mathrm{T}} \boldsymbol{M}\, \boldsymbol{W} = \boldsymbol{M}$, where $\boldsymbol{W}^{\mathrm{T}}$ is the transpose of $\boldsymbol{W}$.

(2) For the *determinant* of $\boldsymbol{W}$, $\det(\boldsymbol{W}) = \pm 1$ must hold; $\det(\boldsymbol{W}) = +1$ for the identity, translations, rotations and screw rotations; $\det(\boldsymbol{W}) = -1$ for inversions, reflections, glide reflections and rotoinversions.

(3) For the *trace*, $\mathrm{tr}(\boldsymbol{W}) = W_{11} + W_{22} + W_{33} = \pm(1 + 2\cos\varphi)$ holds, where φ is the rotation angle; the $+$ sign applies if $\det(\boldsymbol{W}) = +1$ and the $-$ sign if $\det(\boldsymbol{W}) = -1$.

Algorithms for the determination of the kind of isometry from a given matrix–column pair and for the determination of the matrix–column pair for a given isometry can be found in *IT* A, Part 11 or in Hahn & Wondratschek (1994).

1.2.2.6. *Vectors and vector coefficients*

In crystallography, vectors and their coefficients as well as points and their coordinates are used for the description of crystal structures. Vectors represent translation shifts, distance and Patterson vectors, reciprocal-lattice vectors *etc*. With respect to a given basis a vector has three coefficients. In contrast to the coordinates of a point, these coefficients do not change if the origin of the coordinate system is shifted. In the usual description by columns, the vector coefficients cannot be distinguished from the point coordinates, but in the augmented-column description the difference becomes visible: the vector from the point P to the point Q has the coefficients $v_1 = q_1 - p_1$, $v_2 = q_2 - p_2$, $v_3 = q_3 - p_3$, $1 - 1$. Thus, the column of the coefficients of a vector is not augmented by '1' but by '0'. Therefore, when the point P is mapped onto the point $\tilde{P}$ by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ according to equation (1.2.2.3), then the vector $\mathbf{v} = \overrightarrow{PQ}$ is mapped onto the vector $\tilde{\mathbf{v}} = \overrightarrow{\tilde{P}\tilde{Q}}$ by transforming its coefficients by $\tilde{\boldsymbol{v}} = \boldsymbol{W}\boldsymbol{v}$, because the coefficients w_j are multiplied by the number '0' augmenting the column $\boldsymbol{v} = (v_j)$. Indeed, the distance vector $\mathbf{v} = \overrightarrow{PQ}$ is not changed when the whole space is mapped onto itself by a translation.

Remarks:

(1) The difference in transformation behaviour between the point coordinates $\boldsymbol{x}$ and the vector coefficients $\boldsymbol{v}$ is not visible in the equations where the symbols $\mathbb{x}$ and $\mathbb{v}$ are used, but is obvious only if the columns are written in full, *viz*

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \hline 1 \end{pmatrix} \text{ and } \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \hline 0 \end{pmatrix}.$$

(2) The transformation behaviour of the vector coefficients is also apparent if the vector is understood to be a translation vector and the transformation behaviour of the translation is considered as in the last paragraph of the next section.

(3) The transformation $\tilde{\boldsymbol{v}} = \boldsymbol{W}\boldsymbol{v}$ is called an *orthogonal mapping* if $\boldsymbol{W}$ is the matrix part of an isometry.

1.2.2.7. *Origin shift and change of the basis*

It is in general advantageous to refer crystallographic objects and their symmetries to the most appropriate coordinate system. The best coordinate system may be different for different steps of the calculations and for different objects which have to be considered simultaneously. Therefore, a change of the origin and/or the basis are frequently necessary when treating crystallographic problems. Here the formulae for the influence of an origin shift and a change of basis on the coordinates, on the matrix–column pairs of mappings and on the vector coefficients are only stated; the equations are derived in detail in *IT* A Chapters 5.2 and 5.3, and in Hahn & Wondratschek (1994).

Let a coordinate system be given with a basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}}$ and an origin O.[1] Referred to this coordinate system, the column of coordinates of a point P is $\boldsymbol{x}$; the matrix and column parts describing a symmetry operation are $\boldsymbol{W}$ and $\boldsymbol{w}$ according to equations (1.2.2.1) to (1.2.2.3), and the column of vector coefficients is $\boldsymbol{v}$, see Section 1.2.2.6. A new coordinate system may be introduced with the basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\mathrm{T}}$ and the origin O'. Referred to the new coordinate system, the column of coordinates of the point P is $\boldsymbol{x}'$, the symmetry operation is described by $\boldsymbol{W}'$ and $\boldsymbol{w}'$ and the column of vector coefficients is $\boldsymbol{v}'$.

Let $\boldsymbol{p} = \overrightarrow{OO'}$ be the column of coefficients for the vector from the old origin O to the new origin O' and let

$$\boldsymbol{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \qquad (1.2.2.9)$$

be the matrix of a basis change, *i.e.* the matrix that relates the new basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\mathrm{T}}$ to the old basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}}$ according to

$$(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)^{\mathrm{T}} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}} \boldsymbol{P} = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)^{\mathrm{T}} \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}. \qquad (1.2.2.10)$$

[1] In this volume, point coordinates and vector coefficients are thought of as columns in matrix multiplication. Therefore, columns are considered to be 'standard'. These 'columns' are not marked, even if they are written in a row. To comply with the rules of matrix multiplication, rows are also introduced. These rows of symbols (*e.g.* vector coefficients of reciprocal space, *i.e.* Miller indices, or a set of basis vectors of direct space) are 'transposed relative to columns' and are, therefore, marked $(h, k, l)^{\mathrm{T}}$ or $(\mathbf{a}, \mathbf{b}, \mathbf{c})^{\mathrm{T}}$, even if they are written in a row.

Then the following equations hold:

$$\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} - \boldsymbol{P}^{-1}\boldsymbol{p} \text{ or } \boldsymbol{x} = \boldsymbol{P}\boldsymbol{x}' + \boldsymbol{p}; \qquad (1.2.2.11)$$

$$\boldsymbol{W}' = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \text{ or } \boldsymbol{W} = \boldsymbol{P}\boldsymbol{W}'\boldsymbol{P}^{-1}; \qquad (1.2.2.12)$$

$$\boldsymbol{w}' = \boldsymbol{P}^{-1}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}) \text{ or } \boldsymbol{w} = \boldsymbol{P}\boldsymbol{w}' - (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}. \qquad (1.2.2.13)$$

For the columns of vector coefficients $\boldsymbol{v}$ and $\boldsymbol{v}'$, the following holds:

$$\boldsymbol{v}' = \boldsymbol{P}^{-1}\boldsymbol{v} \text{ or } \boldsymbol{v} = \boldsymbol{P}\boldsymbol{v}', \qquad (1.2.2.14)$$

i.e. an origin shift does not change the vector coefficients.

These equations read in the augmented-matrix formalism

$$\mathbb{x}' = \mathbb{P}^{-1}\mathbb{x}; \; \mathbb{W}' = \mathbb{P}^{-1}\mathbb{W}\mathbb{P}; \; \mathbb{v}' = \mathbb{P}^{-1}\mathbb{v}. \qquad (1.2.2.15)$$

For the difference in the transformation behaviour of point coordinates and vector coefficients, see the remarks at the end of Section 1.2.2.6. A vector $\mathbf{v}$ can be regarded as a translation vector; its translation is then described by $(\boldsymbol{I}, \boldsymbol{v})$, *i.e.* $\boldsymbol{W} = \boldsymbol{I}$, $\boldsymbol{w} = \boldsymbol{v}$. It can be shown using equation (1.2.2.13) that the translation and thus the translation vector are not changed under an origin shift, $(\boldsymbol{I}, \boldsymbol{p})$, because $(\boldsymbol{I}, \boldsymbol{v})' = (\boldsymbol{I}, \boldsymbol{v})$ holds. Moreover, under a general coordinate transformation the origin shift is not effective: in equation (1.2.2.13) only $\boldsymbol{v}' = \boldsymbol{P}^{-1}\boldsymbol{v}$ remains because of the equality $\boldsymbol{W} = \boldsymbol{I}$.

1.2.3. Groups

Group theory is the proper tool for studying symmetry in science. The symmetry group of an object is the set of all isometries (rigid motions) which map that object onto itself. If the object is a crystal, the isometries which map it onto itself (and also leave it invariant as a whole) are the *crystallographic symmetry operations*.

There is a huge amount of literature on group theory and its applications. The book *Introduction to Group Theory* by Ledermann (1976) is recommended. The book *Symmetry of Crystals. Introduction to International Tables for Crystallography, Vol. A* by Hahn & Wondratschek (1994) describes a way in which the data of *IT* A can be interpreted by means of matrix algebra and elementary group theory. It may also help the reader of this volume.

1.2.3.1. *Some properties of symmetry groups*

The geometric symmetry of any object is described by a group $\mathcal{G}$. The symmetry operations $g_j \in \mathcal{G}$ are the group elements, and the set $\{g_j \in \mathcal{G}\}$ of all symmetry operations fulfils the group postulates. [A 'symmetry element' in crystallography is not a group element of a symmetry group but is a combination of a geometric object with that set of symmetry operations which leave the geometric object invariant, *e.g.* an axis with its threefold rotations or a plane with its glide reflections *etc.*, *cf.* Flack *et al.* (2000).] Groups will be designated by upper-case calligraphic script letters $\mathcal{G}$, $\mathcal{H}$ *etc*. Group elements are represented by lower-case slanting *sans serif* letters g, h *etc*.

The result g_r of the composition of two elements $g_j, g_k \in \mathcal{G}$ will be called the *product* of g_j and g_k and will be written $g_r = g_k\, g_j$. The first operation is the right factor because the point coordinates or vector coefficients are written as columns on which the matrices of the symmetry operations are applied from the left side.

The *law of composition* in the group is the successive application of the symmetry operations.

The *group postulates* are shown to hold for symmetry groups:

(1) The *closure*, *i.e.* the property that the composition of any two symmetry operations results in a symmetry operation again, is always fulfilled for geometric symmetries: if $g_j \in \mathcal{G}$ and $g_k \in \mathcal{G}$, then $g_j\, g_k = g_r \in \mathcal{G}$ also holds.

(2) The *associative law* is always fulfilled for the composition of geometric mappings. If $g_j, g_k, g_m \in \mathcal{G}$, then $(g_j\, g_k)\, g_m = g_j\,(g_k\, g_m) = g_q$ for any triplet j, k, m. Therefore, the parentheses are not necessary, one can write $g_j\, g_k\, g_m = g_q$. In general, however, the sequence of the symmetry operations must not be changed. Thus, in general $g_j\, g_k\, g_m \neq g_j\, g_m\, g_k$.

(3) The *unit element* or *neutral element* $e \in \mathcal{G}$ is the identity operation which maps each point onto itself, *i.e.* leaves each point invariant.

(4) The isometry which reverses a given symmetry operation $g \in \mathcal{G}$ is also a symmetry operation of $\mathcal{G}$ and is called the *inverse* symmetry operation g^{-1} of g. It has the property $g\, g^{-1} = g^{-1}\, g = e$.

The number of elements of a group $\mathcal{G}$ is called its *order* $|\mathcal{G}|$. The order of a group may be finite, *e.g.* 24 for the symmetry operations of a regular tetrahedron, or infinite, *e.g.* for any space group because of its infinite set of translations. If the relation $g_k\, g_j = g_j\, g_k$ is fulfilled for all pairs of elements of a group $\mathcal{G}$, then $\mathcal{G}$ is called a *commutative* or an *Abelian* group.

For groups of higher order, it is usually inappropriate and for groups of infinite order it is impossible to list all elements of a group. The following definition nearly always reduces the set of group elements to be listed explicitly to a small set.

Definition 1.2.3.1.1. A set $\mathcal{S} = \{g_p,\, g_q,\, \ldots\} \in \mathcal{G}$ such that every element of $\mathcal{G}$ can be obtained by composition of the elements of $\mathcal{S}$ and their inverses is called a *set of generators* of $\mathcal{G}$. The elements $g_i \in \mathcal{S}$ are called *generators* of $\mathcal{G}$. □

A group is *cyclic* if it consists of the unit element e and all powers of one element g:

$$\mathcal{C}(g) = \{\, \ldots\, g^{-3},\, g^{-2},\, g^{-1},\, e,\, g^1,\, g^2,\, g^3,\, \ldots \}.$$

If there is an integer number $n > 0$ with $g^n = e$ and n is the smallest number with this property, then the group $\mathcal{C}(g)$ has the *finite order n*. Let g^{-k} with $0 < k < n$ be the inverse element of g^k where n is the order of g. Because $g^{-k} = g^n\, g^{-k} = g^{n-k} = g^m$ with $n = m + k$, the elements of a cyclic group of finite order can all be written as positive powers of the generator g. Otherwise, if such an integer n does not exist, the group $\mathcal{C}(g)$ is of *infinite order* and the positive powers g^k are different from the negative ones g^{-m}.

In the same way, from any element $g_j \in \mathcal{G}$ its cyclic group $\mathcal{C}(g_j)$ can be generated even if $\mathcal{G}$ is not cyclic itself. The order of this group $\mathcal{C}(g_j)$ is called the *order of the element* g_j.

1.2.3.2. *Group isomorphism and homomorphism*

A finite group $\mathcal{G}$ of small order may be conveniently visualized by its *multiplication table*, *group table* or *Cayley table*. An example is shown in Table 1.2.3.1.

Table 1.2.3.1. *Multiplication table of a group*

The group elements $g \in \mathcal{G}$ are listed at the top of the table and in the same sequence on the left-hand side; the unit element 'e' is listed first. The table is thus a square array. The product $g_k\, g_j$ of any pair of elements is listed at the intersection of the kth row and the jth column.
It can be shown that each group element is listed exactly once in each row and once in each column of the table. In the row of an element $g \in \mathcal{G}$, the unit element e appears in the column of g^{-1}. If $(g)^2 = e$, *i.e.* $g = g^{-1}$, e appears on the main diagonal. The multiplication table of an Abelian group is symmetric about the main diagonal.

$\mathcal{G}$	e	a	b	c	$\ldots$
e	e	a	b	c	$\ldots$
a	a	a^2	ab	ac	$\ldots$
b	b	ba	b^2	bc	$\ldots$
c	c	ca	cb	c^2	$\ldots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

The multiplication tables can be used to define one of the most important relations between two groups, the isomorphism of groups. This can be done by comparing the multiplication tables of the two groups.

Definition 1.2.3.2.1. Two groups are *isomorphic* if one can arrange the rows and columns of their multiplication tables such that these tables are equal, apart from the names or symbols of the group elements. □

Multiplication tables are useful only for groups of small order. To define 'isomorphism' for arbitrary groups, one can formulate the relations expressed by the multiplication tables in a more abstract way.

The 'same multiplication table' for the groups $\mathcal{G}$ and $\mathcal{G}'$ means that there is a reversible mapping $g_q \longleftrightarrow g'_q$ of the elements $g_q \in \mathcal{G}$ and $g'_q \in \mathcal{G}'$ such that $(g_j\, g_k)' = g'_j\, g'_k$ holds for any pair of indices j and k. In words:

Definition 1.2.3.2.2. Two groups $\mathcal{G}$ and $\mathcal{G}'$ are isomorphic if there is a reversible mapping of $\mathcal{G}$ onto $\mathcal{G}'$ such that for any pair of elements of $\mathcal{G}$ the image of the product is equal to the product of the images. □

Isomorphic groups have the same order. By isomorphism the set of all groups is classified into *isomorphism types* or *isomorphism classes* of groups. Such a class is often called an *abstract group*.

The isomorphism between the space groups and the corresponding matrix groups makes an analytical treatment of crystallographic symmetry possible. Moreover, the isomorphism of different space groups allows one to classify the infinite number of space groups into a finite number of *isomorphism types of space groups*, which is one of the bases of crystallography, see Section 1.2.5.

Isomorphism provides a very strong relation between groups: the groups are identical in their group-theoretical properties. One can weaken this relation by omitting the condition of reversibility of the mapping. One then admits that more than one element of the group $\mathcal{G}$ is mapped onto the same element of $\mathcal{G}'$. This concept leads to the definition of homomorphism.

Definition 1.2.3.2.3. A mapping of a group $\mathcal{G}$ onto a group $\mathcal{G}'$ is called *homomorphic*, and $\mathcal{G}'$ is called a *homomorphic image* of the group $\mathcal{G}$, if for any pair of elements of $\mathcal{G}$ the image of the product is equal to the product of the images and if any element of $\mathcal{G}'$ is the image of at least one element of $\mathcal{G}$. The relation of $\mathcal{G}$ and $\mathcal{G}'$ is called a *homomorphism*. More formally: For the mapping $\mathcal{G}$ onto $\mathcal{G}'$, $(g_j\, g_k)' = g'_j\, g'_k$ holds. □

The formulation 'mapping onto' implies that each element $g' \in \mathcal{G}'$ occurs among the images of the elements $g \in \mathcal{G}$ at least once.[2]

The very important concept of homomorphism is discussed further in Lemma 1.2.4.4.3. The crystallographic point groups are homomorphic images of the space groups, see Section 1.2.5.4.

[2] In mathematics, the term 'homomorphism' includes mappings of a group $\mathcal{G}$ *into* a group $\mathcal{G}'$, *i.e.* mappings in which not every $g' \in \mathcal{G}'$ is the image of some element of $g \in \mathcal{G}$. The term 'homomorphism onto' defined above is also known as an *epimorphism*, *e.g.* in Ledermann (1976). In the older literature the term 'multiple isomorphism' can also be found.

1.2.4. Subgroups

1.2.4.1. *Definition*

There may be sets of elements $g_k \in \mathcal{G}$ that do not constitute the full group $\mathcal{G}$ but nevertheless fulfil the group postulates for themselves.

Definition 1.2.4.1.1. A subset $\mathcal{H}$ of elements of a group $\mathcal{G}$ is called a *subgroup* $\mathcal{H}$ of $\mathcal{G}$ if it fulfils the group postulates with respect to the law of composition of $\mathcal{G}$. □

Remarks:

(1) The group $\mathcal{G}$ is considered to be one of its own subgroups. If subgroups $\mathcal{H}_j$ are discussed where $\mathcal{G}$ is included among the subgroups, we write $\mathcal{H}_j \leq \mathcal{G}$ or $\mathcal{G} \geq \mathcal{H}_j$. If $\mathcal{G}$ is excluded from the set $\{\mathcal{H}_j\}$ of its subgroups, we write $\mathcal{H}_j < \mathcal{G}$ or $\mathcal{G} > \mathcal{H}_j$. A subgroup $\mathcal{H}_j < \mathcal{G}$ is called a *proper subgroup* of $\mathcal{G}$.

(2) In a relation $\mathcal{G} \geq \mathcal{H}$ or $\mathcal{G} > \mathcal{H}$, $\mathcal{G}$ is called a *supergroup* of $\mathcal{H}$. The symbols $\leq$, $\geq$, $<$ and $>$ are used for supergroups in the same way as they are used for subgroups, *cf.* Section 2.1.6.

(3) A subgroup of a finite group is finite. A subgroup of an infinite group may be finite or infinite.

(4) A subset $\mathcal{K}$ of elements $g_k \in \mathcal{G}$ which does not necessarily form a group is designated by the symbol $\mathcal{K} \subset \mathcal{G}$.

Definition 1.2.4.1.2. A subgroup $\mathcal{H} < \mathcal{G}$ is a *maximal subgroup* if no group $\mathcal{Z}$ exists for which $\mathcal{H} < \mathcal{Z} < \mathcal{G}$ holds. If $\mathcal{H}$ is a maximal subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a *minimal supergroup* of $\mathcal{H}$. □

This definition is very important for the tables of this volume, as only maximal subgroups of space groups are listed. If all maximal subgroups are known for any given space group, then any general subgroup $\mathcal{H} < \mathcal{G}$ can be obtained by a (finite) chain of maximal subgroups between $\mathcal{G}$ and $\mathcal{H}$, see Section 1.2.6.2. Moreover, the relations between a space group and its maximal subgroups are particularly transparent, *cf.* Lemma 1.2.8.1.3.

1.2.4.2. *Coset decomposition and normal subgroups*

Let $\mathcal{H} < \mathcal{G}$ be a subgroup of $\mathcal{G}$ of order $|\mathcal{H}|$. Because $\mathcal{H}$ is a proper subgroup of $\mathcal{G}$ there must be elements $g_q \in \mathcal{G}$ that are not elements of $\mathcal{H}$. Let $g_2 \in \mathcal{G}$ be one of them. Then the set of elements $g_2\mathcal{H} = \{g_2 h_j \,|\, h_j \in \mathcal{H}\}$[3] is a subset of elements of $\mathcal{G}$ with the property that all its elements are different and that the sets $\mathcal{H}$ and $g_2\mathcal{H}$ have no element in common. Thus, the set $g_2\mathcal{H}$ also contains $|\mathcal{H}|$ elements of $\mathcal{G}$. If there is another element $g_3 \in \mathcal{G}$ which belongs neither to $\mathcal{H}$ nor to $g_2\mathcal{H}$, one can form another set $g_3\mathcal{H} = \{g_3 h_j \,|\, h_j \in \mathcal{H}\}$. All elements of $g_3\mathcal{H}$ are different and none occurs already in $\mathcal{H}$ or in $g_2\mathcal{H}$. This procedure can be continued until each element $g_r \in \mathcal{G}$ belongs to one of these sets. In this way the group $\mathcal{G}$ can be partitioned, such that each element $g \in \mathcal{G}$ belongs to exactly one of these sets.

Definition 1.2.4.2.1. The partition just described is called a *decomposition* $(\mathcal{G} : \mathcal{H})$ *into left cosets* of the group $\mathcal{G}$ relative to the group $\mathcal{H}$. The sets $g_p\mathcal{H}$, $p = 1, \ldots, i$ are called *left cosets*, because the elements $h_j \in \mathcal{H}$ are multiplied with the new elements from the left-hand side. The procedure is called a *decomposition into right cosets* $\mathcal{H}g_s$ if the elements $h_j \in \mathcal{H}$ are multiplied with the new elements g_s from the right-hand side. The elements g_p or g_s are called the *coset representatives*. The number of cosets is called the *index* $i = |\mathcal{G} : \mathcal{H}|$ of $\mathcal{H}$ in $\mathcal{G}$. □

Remarks:

(1) The group $\mathcal{H} = g_1\mathcal{H}$ with $g_1 = e$ is the first coset for both kinds of decomposition. It is the only coset which forms a group by itself.

(2) All cosets have the same *length*, *i.e.* the same number of elements, which is equal to $|\mathcal{H}|$, the order of $\mathcal{H}$.

(3) The index i is the same for both right and left decompositions. In *IT* A and in this volume, the index is frequently designated by the symbol $[i]$.

(4) A coset does not depend on its representative element; starting from any of its elements will result in the same coset. The right cosets may be different from the left ones and the representatives of the right and left cosets may also differ.

(5) If the order $|\mathcal{G}|$ of $\mathcal{G}$ is infinite, then either the order $|\mathcal{H}|$ of $\mathcal{H}$ or the index $i = |\mathcal{G} : \mathcal{H}|$ of $\mathcal{H}$ in $\mathcal{G}$ or both are infinite.

(6) The coset decomposition of a space group $\mathcal{G}$ relative to its translation subgroup $\mathcal{T}(\mathcal{G})$ is fundamental in crystallography, *cf.* Section 1.2.5.4.

From its definition and from the properties of the coset decomposition mentioned above, one immediately obtains the fundamental theorem of Lagrange (for another formulation, see Chapter 1.5):

Lemma 1.2.4.2.2. *Lagrange's theorem*: Let $\mathcal{G}$ be a group of finite order $|\mathcal{G}|$ and $\mathcal{H} < \mathcal{G}$ a subgroup of $\mathcal{G}$ of order $|\mathcal{H}|$. Then $|\mathcal{H}|$ is a divisor of $|\mathcal{G}|$ and the equation $|\mathcal{H}| \times i = |\mathcal{G}|$ holds where $i = |\mathcal{G} : \mathcal{H}|$ is the index of $\mathcal{H}$ in $\mathcal{G}$. □

A special situation exists when the left and right coset decompositions of $\mathcal{G}$ relative to $\mathcal{H}$ result in the partition of $\mathcal{G}$ into the same cosets:

$$g_p\mathcal{H} = \mathcal{H}g_p \text{ for all } 1 \leq p \leq i. \qquad (1.2.4.1)$$

Subgroups $\mathcal{H}$ that fulfil equation (1.2.4.1) are called 'normal subgroups' according to the following definition:

Definition 1.2.4.2.3. A subgroup $\mathcal{H} < \mathcal{G}$ is called a *normal subgroup* or *invariant subgroup* of $\mathcal{G}$, $\mathcal{H} \lhd \mathcal{G}$, if equation (1.2.4.1) is fulfilled. □

The relation $\mathcal{H} \lhd \mathcal{G}$ always holds for $|\mathcal{G} : \mathcal{H}| = 2$, *i.e.* subgroups of index 2 are always normal subgroups. The subgroup $\mathcal{H}$ contains half of the elements of $\mathcal{G}$, whereas the other half of the elements forms 'the other' coset. This coset must then be the right as well as the left coset.

1.2.4.3. *Conjugate elements and conjugate subgroups*

In a coset decomposition, the set of all elements of the group $\mathcal{G}$ is partitioned into cosets which form classes in the mathematical sense of the word, *i.e.* each element of $\mathcal{G}$ belongs to exactly one coset.

Another equally important partition of the group $\mathcal{G}$ into classes of elements arises from the following definition:

Definition 1.2.4.3.1. Two elements $g_j, g_k \in \mathcal{G}$ are called *conjugate* if there is an element $g_q \in \mathcal{G}$ such that $g_q^{-1} g_j\, g_q = g_k$. □

Remarks:

(1) Definition 1.2.4.3.1 partitions the elements of $\mathcal{G}$ into classes of conjugate elements which are called *conjugacy classes of elements*.

(2) The unit element always forms a conjugacy class by itself.

[3] The formulation $g_2\mathcal{H} = \{g_2 h_j \,|\, h_j \in \mathcal{H}\}$ means: '$g_2\mathcal{H}$ is the set of the products $g_2 h_j$ of g_2 with all elements $h_j \in \mathcal{H}$.'

(3) Each element of an Abelian group forms a conjugacy class by itself.
(4) Elements of the same conjugacy class have the same order.
(5) Different conjugacy classes may contain different numbers of elements, *i.e.* have different 'lengths'.

Not only the individual elements of a group $\mathcal{G}$ but also the subgroups of $\mathcal{G}$ can be classified in conjugacy classes.

Definition 1.2.4.3.2. Two subgroups $\mathcal{H}_j, \mathcal{H}_k < \mathcal{G}$ are called *conjugate* if there is an element $g_q \in \mathcal{G}$ such that $g_q^{-1}\mathcal{H}_j\, g_q = \mathcal{H}_k$ holds. This relation is often written $\mathcal{H}_j^{g_q} = \mathcal{H}_k$. □

Remarks:

(1) The 'trivial subgroup' $\mathcal{I}$ (consisting only of the unit element of $\mathcal{G}$) and the group $\mathcal{G}$ itself each form a conjugacy class by themselves.
(2) Each subgroup of an Abelian group forms a conjugacy class by itself.
(3) Subgroups in the same conjugacy class are isomorphic and thus have the same order.
(4) Different conjugacy classes of subgroups may contain different numbers of subgroups, *i.e.* have different lengths.

Equation (1.2.4.1) can be written

$$\mathcal{H} = g_p^{-1}\mathcal{H}\, g_p \text{ or } \mathcal{H} = \mathcal{H}^{g_p} \text{ for all } p;\ 1 \le p \le i. \qquad (1.2.4.2)$$

Using conjugation, Definition 1.2.4.2.3 can be formulated as

Definition 1.2.4.3.3. A subgroup $\mathcal{H}$ of a group $\mathcal{G}$ is a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ if it is identical with all of its conjugates, *i.e.* if its conjugacy class consists of the one subgroup $\mathcal{H}$ only. □

1.2.4.4. *Factor groups and homomorphism*

For the following definition, the 'product of sets of group elements' will be used:

Definition 1.2.4.4.1. Let $\mathcal{G}$ be a group and $\mathcal{K}_j = \{g_{j_1}, \ldots, g_{j_n}\}$, $\mathcal{K}_k = \{g_{k_1}, \ldots, g_{k_m}\}$ be two arbitrary sets of its elements which are not necessarily groups themselves. Then the product $\mathcal{K}_j\,\mathcal{K}_k$ of $\mathcal{K}_j$ and $\mathcal{K}_k$ is the set of all products $\mathcal{K}_j\,\mathcal{K}_k = \{g_{j_p}\, g_{k_q} \mid g_{j_p} \in \mathcal{K}_j,\ g_{k_q} \in \mathcal{K}_k\}$.[4] □

The coset decomposition of a group $\mathcal{G}$ relative to a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ has a property which makes it particularly useful for displaying the structure of a group.

Consider the coset decomposition with the cosets $\mathcal{S}_j$ and $\mathcal{S}_k$ of a group $\mathcal{G}$ relative to its subgroup $\mathcal{H} < \mathcal{G}$. In general the product $\mathcal{S}_j\,\mathcal{S}_k$ of two cosets, *cf.* Definition 1.2.4.4.1, will not be a coset again. However, if and only if $\mathcal{H} \lhd \mathcal{G}$ is a normal subgroup of $\mathcal{G}$, the product of two cosets is always another coset. This means that for the set of all cosets of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$ there exists a law of composition for which the closure is fulfilled. One can show that the other group postulates are also fulfilled for the cosets and their multiplication if $\mathcal{H} \lhd \mathcal{G}$ holds: there is a neutral element (which is $\mathcal{H}$), for each coset $g\,\mathcal{H} = \mathcal{H}\,g$ the coset $g^{-1}\,\mathcal{H} = \mathcal{H}\,g^{-1}$ forms the inverse element and for the coset multiplication the associative law holds.

Definition 1.2.4.4.2. Let $\mathcal{H} \lhd \mathcal{G}$. The cosets of the decomposition of the group $\mathcal{G}$ relative to the normal subgroup $\mathcal{H} \lhd \mathcal{G}$ form a group with respect to the composition law of coset multiplication. This group is called the *factor group* $\mathcal{G}/\mathcal{H}$. Its order is $|\mathcal{G} : \mathcal{H}|$, *i.e.* the index of $\mathcal{H}$ in $\mathcal{G}$. □

A factor group $\mathcal{F} = \mathcal{G}/\mathcal{H}$ is not necessarily isomorphic to a subgroup $\mathcal{H}_j < \mathcal{G}$.

Factor groups are indispensable for an understanding of the homomorphism of one group onto the other. The relations between a group $\mathcal{G}$ and its homomorphic image are very strong and are expressed by the following lemma:

Lemma 1.2.4.4.3. Let $\mathcal{G}'$ be a homomorphic image of the group $\mathcal{G}$. Then the set of all elements of $\mathcal{G}$ that are mapped onto the unit element $e' \in \mathcal{G}'$ forms a normal subgroup $\mathcal{X}$ of $\mathcal{G}$. The group $\mathcal{G}'$ is isomorphic to the factor group $\mathcal{G}/\mathcal{X}$ and the cosets of $\mathcal{X}$ in $\mathcal{G}$ are mapped onto the elements of $\mathcal{G}'$. The normal subgroup $\mathcal{X}$ is called the *kernel* of the mapping; it forms the unit element of the factor group $\mathcal{G}/\mathcal{X}$. A homomorphic image of $\mathcal{G}$ exists for any normal subgroup of $\mathcal{G}$. □

The most important homomorphism in crystallography is the relation between a space group $\mathcal{G}$ and its homomorphic image, the point group $\mathcal{P}$, where the kernel is the subgroup $\mathcal{T}(\mathcal{G})$ of all translations of $\mathcal{G}$, *cf.* Section 1.2.5.4.

1.2.4.5. *Normalizers*

The concept of the normalizer $\mathcal{N}_\mathcal{G}(\mathcal{H})$ of a group $\mathcal{H} < \mathcal{G}$ in a group $\mathcal{G}$ is very useful for the considerations of the following sections. The size of the conjugacy class of $\mathcal{H}$ in $\mathcal{G}$ is determined by this normalizer.

Let $\mathcal{H} < \mathcal{G}$ and $h_j \in \mathcal{H}$. Then $h_j^{-1}\mathcal{H}h_j = \mathcal{H}$ holds because $\mathcal{H}$ is a group. If $\mathcal{H} \lhd \mathcal{G}$, then $g_k^{-1}\mathcal{H}g_k = \mathcal{H}$ for any $g_k \in \mathcal{G}$. If $\mathcal{H}$ is not a normal subgroup of $\mathcal{G}$, there may nevertheless be elements $g_p \in \mathcal{G},\ g_p \notin \mathcal{H}$ for which $g_p^{-1}\mathcal{H}g_p = \mathcal{H}$ holds. We consider the set of all elements $g_p \in \mathcal{G}$ that have this property.

Definition 1.2.4.5.1. The set of all elements $g_p \in \mathcal{G}$ that map the subgroup $\mathcal{H} < \mathcal{G}$ onto itself by conjugation, $\mathcal{H} = g_p^{-1}\mathcal{H}g_p = \mathcal{H}^{g_p}$, forms a group $\mathcal{N}_\mathcal{G}(\mathcal{H})$, called the *normalizer of* $\mathcal{H}$ *in* $\mathcal{G}$, where $\mathcal{H} \unlhd \mathcal{N}_\mathcal{G}(\mathcal{H}) \le \mathcal{G}$. □

Remarks:

(1) The group $\mathcal{H} < \mathcal{G}$ is a normal subgroup of $\mathcal{G}$, $\mathcal{H} \lhd \mathcal{G}$, if and only if $\mathcal{N}_\mathcal{G}(\mathcal{H}) = \mathcal{G}$.
(2) Let $\mathcal{N}_\mathcal{G}(\mathcal{H}) = \{g_p\}$. One can decompose $\mathcal{G}$ into right cosets relative to $\mathcal{N}_\mathcal{G}(\mathcal{H})$. All elements $g_p\, g_r$ of a right coset $\mathcal{N}_\mathcal{G}(\mathcal{H})\, g_r$ of this decomposition $(\mathcal{G}:\mathcal{N}_\mathcal{G}(\mathcal{H}))$ transform $\mathcal{H}$ into the same subgroup $g_r^{-1}\, g_p^{-1}\,\mathcal{H}\, g_p\, g_r = g_r^{-1}\,\mathcal{H}\, g_r < \mathcal{G}$, which is thus conjugate to $\mathcal{H}$ in $\mathcal{G}$ by g_r.
(3) The elements of different cosets of $(\mathcal{G}:\mathcal{N}_\mathcal{G}(\mathcal{H}))$ transform $\mathcal{H}$ into different conjugates of $\mathcal{H}$. The number of cosets of $\mathcal{N}_\mathcal{G}(\mathcal{H})$ is equal to the index $i_N = |\mathcal{G} : \mathcal{N}_\mathcal{G}(\mathcal{H})|$ of $\mathcal{N}_\mathcal{G}(\mathcal{H})$ in $\mathcal{G}$. Therefore, the number $N_\mathcal{H}$ of conjugates in the conjugacy class of $\mathcal{H}$ is equal to the index i_N and is thus determined by the order of $\mathcal{N}_\mathcal{G}(\mathcal{H})$. From $\mathcal{N}_\mathcal{G}(\mathcal{H}) \ge \mathcal{H}$, $i_N = |\mathcal{G} : \mathcal{N}_\mathcal{G}(\mathcal{H})| \le |\mathcal{G} : \mathcal{H}| = i$ follows. This means that the number of conjugates of a subgroup $\mathcal{H} < \mathcal{G}$ cannot exceed the index $i = |\mathcal{G} : \mathcal{H}|$.
(4) If $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of $\mathcal{G}$, then either $\mathcal{N}_\mathcal{G}(\mathcal{H}) = \mathcal{G}$ and $\mathcal{H} \lhd \mathcal{G}$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{N}_\mathcal{G}(\mathcal{H}) = \mathcal{H}$ and the number of conjugates is equal to the index $i = |\mathcal{G} : \mathcal{H}|$.
(5) For the normalizers of the space groups, see the corresponding part of Section 1.2.6.3.

[4] The right-hand side of this equation is the set of all products $g_r = g_{j_p}g_{k_q}$, where g_{j_p} runs through all elements of $\mathcal{K}_j$ and g_{k_q} through all elements of $\mathcal{K}_k$. Each element g_r is taken only once in the set.

1.2.5. Space groups

1.2.5.1. *Space groups and their description*

The set of all symmetry operations of a three-dimensional crystal pattern, *i.e.* its symmetry group, is the *space group* of this crystal pattern. In a plane, the symmetry group of a two-dimensional crystal pattern is its *plane group*. In the following, the term 'space group' alone will be used and the plane groups are included because they are the space groups of two-dimensional space.

A crystal pattern is a periodic array. This means that there are translations among its symmetry operations. The translations of crystals are small (a few angströms to a few hundred angströms) but cannot be arbitrarily short because of the finite size of the particles in crystal structures. One thus defines for any finite integer n:

Definition 1.2.5.1.1. A group $\mathcal{G}$ of isometries in n-dimensional space is called an n-dimensional space group if

(1) $\mathcal{G}$ contains n linearly independent translations.
(2) There is a minimum length $\delta > 0$ such that the length r of any translation vector is at least $r = \delta$. □

Condition (2) is justified because crystal structures contain atoms of finite size, and it is necessary to avoid infinitely small translations as elements of space groups. Several fundamental properties would not hold without this condition, such as the existence of a lattice of translation vectors and the restriction to only a few rotation angles.

In this volume, only the dimensions $n = 2$ and $n = 3$ will be dealt with. However, the space groups (more precisely, the space-group types, *cf.* Section 1.2.5.3) and other crystallographic items are also known for dimensions $n = 4$ and $n = 5$; the number of the affine space-group types is even known for $n = 6$: 28 927 922 (Plesken & Schulz, 2000).

One of the characteristics of a space group is its translation group. Any space group $\mathcal{G}$ is an infinite group because the number of its translations is already infinite. The set of all translations of $\mathcal{G}$ forms the infinite translation subgroup $\mathcal{T}(\mathcal{G}) \triangleleft \mathcal{G}$ with the composition law of performing one translation after the other, represented by the multiplication of matrix–column pairs. The group $\mathcal{T}(\mathcal{G})$ is a normal subgroup of $\mathcal{G}$ of finite index. The vector lattice **L**, *cf.* Section 1.2.2.2, forms a group with the composition law of vector addition. This group is isomorphic to the group $\mathcal{T}(\mathcal{G})$.

The matrix–column pairs of the symmetry operations of a space group $\mathcal{G}$ are mostly referred to the *conventional coordinate system*. Its basis is chosen as a lattice basis and in such a way that the matrices for the linear parts of the symmetry operations of $\mathcal{G}$ are particularly simple. The origin is chosen such that as many coset representatives as possible can be selected with their column coefficients to be zero, or such that the origin is situated on a centre of inversion. This means (for details and examples see Section 8.3.1 of *IT* A):

(1) The basis is always chosen such that all matrix coefficients are 0 or ±1.
(2) If possible, the basis is chosen such that all matrices have main diagonal form; then six of the nine coefficients are 0 and three are ±1.
(3) If (2) is not possible, the basis is chosen such that the matrices are orthogonal. Again, six coefficients are 0 and three are ±1.
(4) If (3) is not possible, the basis is hexagonal. At least five of the nine matrix coefficients are 0 and at most four are ±1.
(5) The conventional basis chosen according to these rules is not always primitive, *cf.* the first example of Section 8.3.1 of *IT* A. If the conventional basis is primitive, then the lattice is also called *primitive*; if the conventional basis is not primitive, then the lattice referred to this (non-primitive) basis is called a *centred lattice*.
(6) The matrix parts of a translation and of an inversion are

$$\boldsymbol{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \overline{\boldsymbol{I}} = \begin{pmatrix} \overline{1} & 0 & 0 \\ 0 & \overline{1} & 0 \\ 0 & 0 & \overline{1} \end{pmatrix},$$

i.e. the unit matrix and the negative unit matrix. They are independent of the basis.
(7) The basis vectors of a crystallographic basis are lattice vectors. This makes the description of the lattice and of the symmetry operations of a crystal pattern independent of the actual metrics of the lattice, *e.g.* independent of temperature and pressure. It also means that the description of the symmetry may be the same for space groups of the same type, *cf.* Section 1.2.5.3.
(8) The origin is chosen at a point of highest site symmetry which is left invariant by as many symmetry operations as possible. The column parts $\boldsymbol{w}_k$ of these symmetry operations are $\boldsymbol{w}_k = \boldsymbol{o}$, *i.e.* the columns consist of zeroes only.

It is obviously impossible to list all elements of an infinite group individually. One could define the space group by a set of generators, because the number of necessary generators for any space group is finite: theoretically, up to six generators might be necessary but in practice up to ten generators are chosen for a space group. In *IT* A and in this volume, the set of the conventional generators is listed in the block 'Generators selected'. The unit element is taken as the first generator; the generating translations follow and the generation is completed with the generators of the non-translation symmetry operations. The rules for the choice of the conventional generators are described in *IT* A, Section 8.3.5.

The description by generators is particularly important for this volume because many of the maximal subgroups in Chapters 2.2 and 2.3 are listed by their generators. These generators are chosen such that the generation of the general position can follow a *composition series*, *cf.* Ledermann (1976). This procedure allows the generation by a short program or even by hand. For details see *IT* A, Section 8.3.5; in Table 8.3.5.2 of *IT* A an example for the generation of a space group along these lines is displayed.

There are four ways to describe a space group in *IT* A:

(i) A set of generators is the first way in which the space-group types $\mathcal{G}$, *cf.* Section 1.2.5.3, are described in *IT* A. This way is also used in the tables of this volume.
(ii) By the matrices of the coset representatives of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ in the general position. These matrices are not written in full but in a shorthand notation, *cf.* Section 8.1.5 or Chapter 11.1 of *IT* A. This kind of description is used for *translationengleiche* maximal subgroups in Chapters 2.2 and 2.3 of this volume, but in a slightly modified way, *cf.* Section 2.1.3.
(iii) In a visual way by diagrams of the symmetry elements (not symmetry operations!) of $\mathcal{G}$ within a unit cell and its surroundings.
(iv) Also in a visual way by depicting the general-position points, again within a unit cell and its surroundings.

1.2.5.2. *Classifications of space groups*

There are an infinite number of space groups because there are an infinite number of known or conceivable crystals and crystal patterns. Indeed, because the lattice parameters depend on temperature and pressure, so do the lattice translations and the space group of a crystal. There is great interest in getting an overview of this vast number of space groups. To achieve this goal, one first characterizes the space groups by their group-theoretical properties and classifies them into space-group types where the space groups of each type have certain properties in common. To get a better overview, one then classifies the space-group types such that related types belong to the same 'superclass'. This classification is done in two ways (*cf.* Sections 1.2.5.4 and 1.2.5.5):

(1) first into *geometric crystal classes* by the point group of the space group, and then into *crystal systems*;
(2) into the arithmetic crystal classes of the space groups and then into *Bravais flocks* and into *lattice systems* (not treated here, *cf. IT* A, Section 8.2.5);
(3) all these classes: geometric and arithmetic crystal classes, crystal systems, Bravais flocks and lattice systems are classified into *crystal families*.

In reality, the tables in Chapters 2.2 and 2.3 and the graphs in Chapters 2.4 and 2.5 are tables and graphs for space-group types. The sequence of the space-group types in *IT* A and thus in this volume is determined by their crystal class, their crystal system and their crystal family. Therefore, these classifications are treated in the next sections. The point groups and the translation groups of the space groups can also be classified in a similar way. Only the classification of the point groups is treated in this chapter. For a more detailed treatment and for the classification of the lattices, the reader is referred to Chapter 1.5 of this volume, to Part 8 of *IT* A or to Brown *et al.* (1978).

1.2.5.3. *Space groups and space-group types*

We first consider the classification of the space groups into types. A more detailed treatment may be found in Section 8.2.1 of *IT* A. In practice, a common way is to look for the symmetry of the space group $\mathcal{G}$ and to compare this symmetry with that of the diagrams in the tables of *IT* A.

With the exception of some double descriptions,[5] there is exactly one set of diagrams which displays the symmetry of $\mathcal{G}$, and $\mathcal{G}$ belongs to that space-group type which is described in this set. From those diagrams the Hermann–Mauguin symbol, abbreviated as HM symbol, the Schoenflies symbol and the space-group number are taken.

A rigorous definition is:

Definition 1.2.5.3.1. Two space groups belong to the same *affine space-group type* if and only if they are isomorphic.[6] □

This definition refers to a rather abstract property which is of great mathematical but less practical value. In crystallography another definition is more appropriate which results in exactly the same space-group types as are obtained by isomorphism. It starts from the description of the symmetry operations of a space group by matrix–column pairs or, as will be formulated here, by augmented matrices. For this one refers each of the space groups to one of its lattice bases.

Definition 1.2.5.3.2. Two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same *affine space-group type* if for a lattice basis and an origin of $\mathcal{G}$, a lattice basis and an origin of $\mathcal{G}'$ can also be found so that the groups of augmented matrices $\{\mathbb{W}\}$ describing $\mathcal{G}$ and $\{\mathbb{W}'\}$ describing $\mathcal{G}'$ are identical. □

In this definition the coordinate systems are chosen such that the groups of augmented matrices agree. It is thus possible to describe the symmetry of all space groups of the same type by one (standardized) set of matrix–column pairs, as is done, for example, in the tables of *IT* A.

In the subgroup tables of Chapters 2.2 and 2.3 it frequently happens that a subgroup $\mathcal{H} < \mathcal{G}$ of a space group $\mathcal{G}$ is given by its matrix–column pairs referred to an nonconventional coordinate system. In this case, a transformation of the coordinate system can bring the matrix–column pairs to the standard form by which the space-group type may be determined. In the subgroup tables both the space-group type and the transformation of the coordinate system are listed. One can also use this procedure for the definition of the term 'affine space-group type':

Definition 1.2.5.3.3. Let two space groups $\mathcal{G}$ and $\mathcal{G}'$ be referred to lattice bases and represented by their groups of augmented matrices $\{\mathbb{W}\}$ and $\{\mathbb{W}'\}$. The groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same *affine space-group type* if an augmented matrix $\mathbb{P}$ with linear part $\boldsymbol{P}$, $\det(\boldsymbol{P}) \neq 0$, and column part $\boldsymbol{p}$ exists, for which

$$\{\mathbb{W}'\} = \mathbb{P}^{-1}\,\{\mathbb{W}\}\,\mathbb{P} \qquad (1.2.5.1)$$

holds. □

The affine space-group types are classes in the mathematical sense of the word, *i.e.* each space group belongs to exactly one type. The derivation of these types reveals 219 affine space-group types and 17 plane-group types.

In crystallography one usually distinguishes 230 rather than 219 space-group types in a slightly finer subdivision. The difference can best be explained using Definition 1.2.5.3.3. The matrix part $\boldsymbol{P}$ may have a negative determinant. In this case, a right-handed basis is converted into a left-handed one, and right-handed and left-handed screw axes are exchanged. It is a convention in crystallography to always refer the space to a right-handed basis and hence transformations with $\det(\boldsymbol{P}) < 0$ are not admitted.

Definition 1.2.5.3.4. If the matrix $\boldsymbol{P}$ is restricted by the condition $\det(\boldsymbol{P}) > 0$, 11 affine space-group types split into two space-group types each, one with right-handed and one with left-handed screw axes, such that the total number of types is 230. These 230 space-group types are called *crystallographic space-group types*. The 11 splitting space-group types are called *pairs of enantiomorphic space-group types* and the space groups themselves are enantiomorphic pairs of space groups. □

The space groups of an enantiomorphic pair belong to different crystallographic space-group types but are isomorphic. As a consequence, in the lists of isomorphic subgroups $\mathcal{H} < \mathcal{G}$ of the tables of Chapter 2.3, there may occur subgroups $\mathcal{H}$ with another conventional HM symbol and another space-group number than that of $\mathcal{G}$, *cf.* Example 1.2.6.2.7. In such a case, $\mathcal{G}$ and $\mathcal{H}$ are members of an enantiomorphic pair of space groups and $\mathcal{H}$ belongs to the space-group type enantiomorphic to that of $\mathcal{G}$. There are no enantiomorphic pairs of plane groups.

[5] Monoclinic space groups are described in the settings 'unique axis *b*' and 'unique axis *c*'; rhombohedral space groups are described in the settings 'hexagonal axes' and 'rhombohedral axes'; and 24 space groups are described with two origins by 'origin choice 1' and 'origin choice 2'. In each case, both descriptions lead to the same short Hermann–Mauguin symbol and space-group number.

[6] The name 'affine space-group type' stems from Definition 1.2.5.3.3. 'Affine space-group types' have to be distinguished from 'crystallographic space-group types' which are defined by Definition 1.2.5.3.4.

The space groups are of different complexity. The simplest ones are the symmorphic space groups (not to be confused with 'isomorphic' space groups) according to the following definition:

Definition 1.2.5.3.5. A space group $\mathcal{G}$ is called *symmorphic* if representatives g_k of all cosets $\mathcal{T}(\mathcal{G})\, g_k$ can be found such that the set $\{g_k\}$ of all representatives forms a group. □

The group $\{g_k\}$ is finite and thus leaves a point F fixed. In the standard setting of any symmorphic space group such a point F is chosen as the origin. Thus, the translation parts of the elements g_k consist of zeroes only.

If a space group is symmorphic then all space groups of its type are symmorphic. Therefore, one can speak of 'symmorphic space-group types'. Symmorphic space groups can be recognized easily by their HM symbols: they contain an unmodified point-group symbol: rotations, reflections, inversions and rotoinversions but no screw rotations or glide reflections. There are 73 symmorphic space-group types of dimension three and 13 of dimension two; none of them show enantiomorphism.

One frequently speaks of 'the 230 space groups' or 'the 17 plane groups' and does not distinguish between the terms 'space group' and 'space-group type'. This is very often possible and is also done in this volume in order to make the explanations less long-winded. However, occasionally the distinction is indispensable in order to avoid serious difficulties of comprehension. For example, the sentence 'A space group is a proper subgroup of itself' is incomprehensible, whereas the sentence 'A space group and its proper subgroup belong to the same space-group type' makes sense.

1.2.5.4. *Point groups and crystal classes*

If the point coordinates are mapped by an isometry and its matrix–column pair, the vector coefficients are mapped by the linear part, *i.e.* by the matrix alone, *cf.* Section 1.2.2.6. Because the number of its elements is infinite, a space group generates from one point an infinite set of symmetry-equivalent points by its matrix–column pairs. Because the number of matrices of the linear parts is finite, the group of matrices generates from one vector a finite set of symmetry-equivalent vectors, *e.g.* the vectors normal to certain planes of the crystal. These planes determine the morphology of the ideal macroscopic crystal and its cleavage; the centre of the crystal represents the zero vector. When the symmetry of a crystal can only be determined by its macroscopic properties, only the symmetry group of the macroscopic crystal can be found. All its symmetry operations leave at least one point of the crystal fixed, *viz* its centre of mass. Therefore, this symmetry group was called the *point group of the crystal*, although its symmetry operations are those of vector space, not of point space. Although misunderstandings are not rare, this name is still used in today's crystallography for historical reasons.[7]

Let a conventional coordinate system be chosen and the elements $g_j \in \mathcal{G}$ be represented by the matrix–column pairs $(\boldsymbol{W}_j, \boldsymbol{w}_j)$, with the representation of the translations $t_k \in \mathcal{T}(\mathcal{G})$ by the pairs $(\boldsymbol{I}, \boldsymbol{t}_k)$. Then the composition of $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ with all translations forms an infinite set $\{(\boldsymbol{I}, \boldsymbol{t}_k)\,(\boldsymbol{W}_j, \boldsymbol{w}_j) = (\boldsymbol{W}_j, \boldsymbol{w}_j + \boldsymbol{t}_k)\}$ of symmetry operations which is a right coset of the coset decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$. From this equation it follows that the elements of the same coset of the decomposition $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ have the same linear part. On the other hand, elements of different cosets have different linear parts if $\mathcal{T}(\mathcal{G})$ contains all translations of $\mathcal{G}$. Thus, each coset can be characterized by its linear part. It can be shown from equations (1.2.2.5) and (1.2.2.6) that the linear parts form a group which is isomorphic to the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, *i.e.* to the group of the cosets.

Definition 1.2.5.4.1. A group of linear parts, represented by a group of matrices $\boldsymbol{W}_j$, is called a *point group* $\mathcal{P}$. If the linear parts are those of the matrix–column pairs describing the symmetry operations of a space group $\mathcal{G}$, the group is called the *point group* $\mathcal{P}_{\mathcal{G}}$ of the space group $\mathcal{G}$. The point groups that can belong to space groups are called *crystallographic point groups*. □

According to Definition 1.2.5.4.1, the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is isomorphic to the point group $\mathcal{P}_{\mathcal{G}}$. This property is exploited in the graphs of *translationengleiche* subgroups of space groups, *cf.* Chapter 2.4 and Section 2.1.7.2.

All point groups in the following sections are crystallographic point groups. The maximum order of a crystallographic point group is 48 in three-dimensional space and 12 in two-dimensional space.

As with space groups, there are also an infinite number of crystallographic point groups which may be classified into a finite number of point-group types. This cannot be done by isomorphism because geometrically different point groups may be isomorphic. For example, point groups consisting of the identity with the inversion $\{\boldsymbol{I}, \overline{\boldsymbol{I}}\}$ or with a twofold rotation $\{\boldsymbol{I}, \boldsymbol{2}\}$ or with a reflection through a plane $\{\boldsymbol{I}, \boldsymbol{m}\}$ are all isomorphic to the (abstract) group of order 2. As for space groups, the classification may be performed, however, referring the point groups to corresponding vector bases. As translations do not occur among the point-group operations, one may choose any basis for the description of the symmetry operations by matrices. One takes the basis of $\{\boldsymbol{W}'\}$ as given and transforms the basis of $\{\boldsymbol{W}\}$ to the basis corresponding to that of $\{\boldsymbol{W}'\}$. This leads to the definition:

Definition 1.2.5.4.2. Two crystallographic point groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}'_{\mathcal{G}'}$ belong to the same *point-group type* or to the same *crystal class of point groups* if there is a real non-singular matrix $\boldsymbol{P}$ which maps a matrix group $\{\boldsymbol{W}\}$ of $\mathcal{P}_{\mathcal{G}}$ onto a matrix group $\{\boldsymbol{W}'\}$ of $\mathcal{P}'_{\mathcal{G}'}$ by the transformation $\{\boldsymbol{W}'\} = \boldsymbol{P}^{-1}\,\{\boldsymbol{W}\}\,\boldsymbol{P}$. □

Point groups can be classified by Definition 1.2.5.4.2. Further space groups may be classified into 'crystal classes of space groups' according to their point groups:

Definition 1.2.5.4.3. Two space groups belong to the same *crystal class of space groups* if their point groups belong to the same crystal class of point groups. □

Whether two space groups belong to the same crystal class or not can be worked out from their standard HM symbols: one removes the lattice parts from these symbols as well as the constituents '1' from the symbols of trigonal space groups and replaces all constituents for screw rotations and glide reflections by those for the corresponding pure rotations and reflections. The symbols obtained in this way are those of the corresponding point groups. If they agree, the space groups belong to the same crystal class. The space groups also belong to the same crystal class if the point-group symbols belong to the pair $\overline{4}2m$ and $\overline{4}m2$ or to the pair $\overline{6}2m$ and $\overline{6}m2$.

There are 32 classes of three-dimensional crystallographic point groups and 32 crystal classes of space groups, and ten classes of two-dimensional crystallographic point groups and ten crystal classes of plane groups.

The distribution into crystal classes classifies space-group types – and thus space groups – and crystallographic point groups. It

[7] The term *point group* is also used for a group of symmetry operations of point space, which is better called a *site-symmetry group* and which is the group describing the symmetry of the surroundings of a point in point space.

does not classify the infinite set of all lattices into a finite number of lattice types, because the same lattice may belong to space groups of different crystal classes. For example, the same lattice may be that of a space group of type $P1$ (of crystal class 1) and that of a space group of type $P\overline{1}$ (of crystal class $\overline{1}$).

Nevertheless, there is also a definition of the 'point group of a lattice'. Let a vector lattice $\mathbf{L}$ of a space group $\mathcal{G}$ be referred to a lattice basis. Then the linear parts $\boldsymbol{W}$ of the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ of $\mathcal{G}$ form the point group $\mathcal{P}_{\mathcal{G}}$. If $(\boldsymbol{W}, \boldsymbol{w})$ maps the space group $\mathcal{G}$ onto itself, then the linear part $\boldsymbol{W}$ maps the (vector) lattice $\mathbf{L}$ onto itself. However, there may be additional matrices which also describe symmetry operations of the lattice $\mathbf{L}$. For example, the point group $\mathcal{P}_{\mathcal{G}}$ of a space group of type $P1$ consists of the identity $\boldsymbol{I}$ only. However, with any vector $\mathbf{t} \in \mathbf{L}$, the negative vector $-\mathbf{t} \in \mathbf{L}$ also belongs to $\mathbf{L}$. Therefore, the lattice $\mathbf{L}$ is always centrosymmetric and has the inversion $\overline{\boldsymbol{I}}$ as a symmetry operation independent of the symmetry of the space group.

Definition 1.2.5.4.4. The set of all orthogonal mappings with matrices $\boldsymbol{W}$ which map a lattice $\mathbf{L}$ onto itself is called the point group of the lattice $\mathbf{L}$ or the *holohedry* of the lattice $\mathbf{L}$. A crystal class of point groups $\mathcal{P}_{\mathcal{G}}$ is called a *holohedral crystal class* if it contains a holohedry. □

There are seven holohedral crystal classes in the space: $\overline{1}$, $2/m$, mmm, $4/mmm$, $\overline{3}m$, $6/mmm$ and $m\overline{3}m$. Their lattices are called triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal and cubic, respectively. There are four holohedral crystal classes in the plane: 2, $2mm$, $4mm$ and $6mm$. Their two-dimensional lattices (or nets) are called oblique, rectangular, square and hexagonal, respectively.

The lattices can be classified into *lattice types* or *Bravais types*, mostly called *Bravais lattices*, or into *lattice systems* (called *Bravais systems* in editions 1 to 4 of *IT* A). These classifications are not discussed here because they are not directly relevant to the classification of the space groups. This is because the lattice symmetry is not necessarily typical for the symmetry of its space group but may accidentally be higher. For example, the lattice of a monoclinic crystal may be accidentally orthorhombic (only for certain values of temperature and pressure). In Sections 8.2.5 and 8.2.7 of *IT* A the 'typical lattice symmetry' of a space group is defined.

1.2.5.5. *Crystal systems and crystal families*

The example of $P1$ mentioned above shows that the point group of the lattice may be systematically of higher order than that of its space group. There are obviously point groups and thus space groups that belong to a holohedral crystal class and those that do not. The latter can be assigned to a holohedral crystal class uniquely according to the following definition:[8]

Definition 1.2.5.5.1. A crystal class $\mathbf{C}$ of a space group $\mathcal{G}$ is either holohedral $\mathbf{H}$ or it can be assigned uniquely to $\mathbf{H}$ by the condition: any point group of $\mathbf{C}$ is a subgroup of a point group of $\mathbf{H}$ but not a subgroup of a holohedral crystal class $\mathbf{H}'$ of smaller order. The set of all crystal classes of space groups that are assigned to the same holohedral crystal class is called a *crystal system* of space groups. □

The 32 crystal classes of space groups are classified into seven crystal systems which are called *triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic*. There are four crystal systems of plane groups: *oblique, rectangular, square and hexagonal*. Like the space groups, the crystal classes of point groups are classified into the seven crystal systems of point groups.

Apart from accidental lattice symmetries, the space groups of different crystal systems have lattices of different symmetry. As an exception, the hexagonal primitive lattice occurs in both hexagonal and trigonal space groups as the typical lattice. Therefore, the space groups of the trigonal and the hexagonal crystal systems are more related than space groups from other different crystal systems. Indeed, in different crystallographic schools the term 'crystal system' was used for different objects. One sense of the term was the 'crystal system' as defined above, while another sense of the old term 'crystal system' is now called a 'crystal family' according to the following definition [for definitions that are also valid in higher-dimensional spaces, see Brown *et al.* (1978) or *IT* A, Chapter 8.2]:

Definition 1.2.5.5.2. In three-dimensional space, the classification of the set of all space groups into crystal families is the same as that into crystal systems with the one exception that the trigonal and hexagonal crystal systems are united to form the *hexagonal crystal family*. There is no difference between crystal systems and crystal families in the plane. □

The partition of the space groups into crystal families is the most universal one. The space groups and their types, their crystal classes and their crystal systems are classified by the crystal families. Analogously, the crystallographic point groups and their crystal classes and crystal systems are classified by the crystal families of point groups. Lattices, their Bravais types and lattice systems can also be classified into crystal families of lattices; *cf. IT* A, Chapter 8.2.

1.2.6. Types of subgroups of space groups

1.2.6.1. *Introductory remarks*

Group–subgroup relations form an essential part of the applications of space-group theory. Let $\mathcal{G}$ be a space group and $\mathcal{H} < \mathcal{G}$ a proper subgroup of $\mathcal{G}$. All maximal subgroups $\mathcal{H} < \mathcal{G}$ of any space group $\mathcal{G}$ are listed in Part 2 of this volume. There are different kinds of subgroups which are defined and described in this section. The tables and graphs of this volume are arranged according to these kinds of subgroups. Moreover, for the different kinds of subgroups different data are listed in the subgroup tables and graphs.

Let $\mathcal{G}_j$ and $\mathcal{H}_j$ be space groups of the space-group types $\mathcal{G}$ and $\mathcal{H}$. The group–subgroup relation $\mathcal{G}_j > \mathcal{H}_j$ is a relation between the particular space groups $\mathcal{G}_j$ and $\mathcal{H}_j$ but it can be generalized to the space-group types $\mathcal{G}$ and $\mathcal{H}$. Certainly, not every space group of the type $\mathcal{H}$ will be a subgroup of every space group of the type $\mathcal{G}$. Nevertheless, the relation $\mathcal{G}_j > \mathcal{H}_j$ holds for any space group of $\mathcal{G}$ and $\mathcal{H}$ in the following sense: If $\mathcal{G}_j > \mathcal{H}_j$ holds for the pair $\mathcal{G}_j$ and $\mathcal{H}_j$, then for any space group $\mathcal{G}_k$ of the type $\mathcal{G}$ a space group $\mathcal{H}_k$ of the type $\mathcal{H}$ exists for which the corresponding relation $\mathcal{G}_k > \mathcal{H}_k$ holds. Conversely, for any space group $\mathcal{H}_m$ of the type $\mathcal{H}$ a space group $\mathcal{G}_m$ of the type $\mathcal{G}$ exists for which the corresponding relation $\mathcal{G}_m > \mathcal{H}_m$ holds. Only this property of the group–subgroup relations made it possible to compile and arrange the tables of this volume so that they are as concise as those of *IT* A.

1.2.6.2. *Definitions and examples*

'Maximal subgroups' have been introduced by Definition 1.2.4.1.2. The importance of this definition will become apparent

[8] This assignment does hold for low dimensions of space at least up to dimension 4. A dimension-independent definition of the concepts of 'crystal system' and 'crystal family' is found in *IT* A, Chapter 8.2, where the classifications are treated in more detail.

in the corollary to Hermann's theorem, *cf.* Lemma 1.2.8.1.3. In this volume only the maximal subgroups are listed for any plane and any space group. A maximal subgroup of a plane group is a plane group, a maximal subgroup of a space group is a space group. On the other hand, a minimal supergroup of a plane group or of a space group is not necessarily a plane group or a space group, *cf.* Section 2.1.6.

If the maximal subgroups are known for each space group, then each non-maximal subgroup of a space group $\mathcal{G}$ with finite index can in principle be obtained from the data on maximal subgroups. A non-maximal subgroup $\mathcal{H} < \mathcal{G}$ of finite index $[i]$ is connected with the original group $\mathcal{G}$ through a chain $\mathcal{H} = \mathcal{Z}_k < \mathcal{Z}_{k-1} < \ldots < \mathcal{Z}_1 < \mathcal{Z}_0 = \mathcal{G}$, where each group $\mathcal{Z}_j < \mathcal{Z}_{j-1}$ is a maximal subgroup of $\mathcal{Z}_{j-1}$, with the index $[i_j] = |\mathcal{Z}_{j-1} : \mathcal{Z}_j|$, $j = 1, \ldots, k$. The number k is finite and the relation $i = \prod_{j=1}^{k} i_j$ holds, *i.e.* the total index $[i]$ is the product of the indices i_j.

According to Hermann (1929), the following types of subgroups of space groups have to be distinguished:

Definition 1.2.6.2.1. A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is called a *translationengleiche subgroup* or a *t*-subgroup of $\mathcal{G}$ if the set $\mathcal{T}(\mathcal{G})$ of translations is retained, *i.e.* $\mathcal{T}(\mathcal{H}) = \mathcal{T}(\mathcal{G})$, but the number of cosets of $\mathcal{G}/\mathcal{T}(\mathcal{G})$, *i.e.* the order P of the point group $\mathcal{P}_\mathcal{G}$, is reduced such that $|\mathcal{G}/\mathcal{T}(\mathcal{G})| > |\mathcal{H}/\mathcal{T}(\mathcal{H})|$.[9] □

The order of a crystallographic point group $\mathcal{P}_\mathcal{G}$ of the space group $\mathcal{G}$ is always finite. Therefore, the number of the subgroups of $\mathcal{P}_\mathcal{G}$ is also always finite and these subgroups and their relations are displayed in well known graphs, *cf.* Chapter 2.4 and Section 2.1.7 of this volume. Because of the isomorphism between the point group $\mathcal{P}_\mathcal{G}$ and the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$, the subgroup graph for the point group $\mathcal{P}_\mathcal{G}$ is the same as that for the *t*-subgroups of $\mathcal{G}$, only the labels of the groups are different. For deviations between the point-group graphs and the actual space-group graphs of Chapter 2.4, *cf.* Section 2.1.7.2.

Example 1.2.6.2.2.

Consider a space group $\mathcal{G}$ of type $P12/m1$ referred to a conventional coordinate system. The translation subgroup $\mathcal{T}(\mathcal{G})$ consists of all translations with translation vectors $\mathbf{t} = u\mathbf{a}+v\mathbf{b}+w\mathbf{c}$, where u, v, w run through all integer numbers. The coset decomposition of $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ results in the four cosets $\mathcal{T}(\mathcal{G})$, $\mathcal{T}(\mathcal{G})\,\boldsymbol{2}_0$, $\mathcal{T}(\mathcal{G})\,\boldsymbol{m}_0$ and $\mathcal{T}(\mathcal{G})\,\overline{\boldsymbol{1}}_0$, where the right operations are a twofold rotation $\boldsymbol{2}_0$ around the rotation axis passing through the origin, a reflection $\boldsymbol{m}_0$ through a plane containing the origin and an inversion $\overline{\boldsymbol{1}}_0$ with the inversion point at the origin, respectively. The three combinations $\mathcal{H}_1 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\,\boldsymbol{2}_0$, $\mathcal{H}_2 = \mathcal{T}(\mathcal{G}) \cup \mathcal{T}(\mathcal{G})\,\boldsymbol{m}_0$ and $\mathcal{H}_3 = \mathcal{T}(\mathcal{G}) \cup (\mathcal{T}\mathcal{G})\,\overline{\boldsymbol{1}}_0$ each form a *translationengleiche* maximal subgroup of $\mathcal{G}$ of index 2 with the space-group symbols $P121$, $P1m1$ and $P\overline{1}$, respectively.

Definition 1.2.6.2.3. A subgroup $\mathcal{H} < \mathcal{G}$ of a space group $\mathcal{G}$ is called a *klassengleiche subgroup* or a *k-subgroup* if the set $\mathcal{T}(\mathcal{G})$ of all translations of $\mathcal{G}$ is reduced to $\mathcal{T}(\mathcal{H}) < \mathcal{T}(\mathcal{G})$ but all linear parts of $\mathcal{G}$ are retained. Then the number of cosets of the decompositions $\mathcal{H}/\mathcal{T}(\mathcal{H})$ and $\mathcal{G}/\mathcal{T}(\mathcal{G})$ is the same, *i.e.* $|\mathcal{H}/\mathcal{T}(\mathcal{H})| = |\mathcal{G}/\mathcal{T}(\mathcal{G})|$. In other words: the order of the point group $\mathcal{P}_\mathcal{H}$ is the same as that of $\mathcal{P}_\mathcal{G}$. See also footnote 9. □

For a *klassengleiche* subgroup $\mathcal{H} < \mathcal{G}$, the cosets of the factor group $\mathcal{H}/\mathcal{T}(\mathcal{H})$ are smaller than those of $\mathcal{G}/\mathcal{T}(\mathcal{G})$. Because $\mathcal{T}(\mathcal{H})$ is still infinite, the number of elements of each coset is infinite but the index $|\mathcal{T}(\mathcal{G}) : \mathcal{T}(\mathcal{H})| > 1$ is finite. The number of *k*-subgroups of $\mathcal{G}$ is always infinite.

Example 1.2.6.2.4.

Consider a space group $\mathcal{G}$ of the type $C121$, referred to a conventional coordinate system. The set $\mathcal{T}(\mathcal{G})$ of all translations can be split into the set $\mathcal{T}_i$ of all translations with integer coefficients u, v and w and the set $\mathcal{T}_f$ of all translations for which the coefficients u and v are fractional. The set $\mathcal{T}_i$ forms a group; the set $\mathcal{T}_f$ is the other coset in the decomposition $(\mathcal{T}(\mathcal{G}) : \mathcal{T}_i)$ and does not form a group. Let t_C be the 'centring translation' with the translation vector $\frac{1}{2}(\mathbf{a} + \mathbf{b})$. Then $\mathcal{T}_f$ can be written $\mathcal{T}_i\, t_C$. Let $\boldsymbol{2}_0$ mean a twofold rotation around the rotation axis through the origin. There are altogether four cosets of the decomposition $(\mathcal{G} : \mathcal{T}_i)$, which can be written now as $\mathcal{T}_i$, $\mathcal{T}_f = \mathcal{T}_i\, t_C$, $\mathcal{T}_i\,\boldsymbol{2}_0$ and $\mathcal{T}_f\,\boldsymbol{2}_0 = (\mathcal{T}_i\, t_C)\,\boldsymbol{2}_0 = \mathcal{T}_i\,(t_C\,\boldsymbol{2}_0)$. The union $\mathcal{T}_i \cup (\mathcal{T}_i\, t_C) = \mathcal{T}_\mathcal{G}$ forms the *translationengleiche* maximal subgroup $C1$ (conventional setting $P1$) of $\mathcal{G}$ of index 2. The union $\mathcal{T}_i \cup (\mathcal{T}_i\,\boldsymbol{2}_0)$ forms the *klassengleiche* maximal subgroup $P121$ of $\mathcal{G}$ of index 2. The union $\mathcal{T}_i \cup (\mathcal{T}_i(t_C\,\boldsymbol{2}_0))$ also forms a *klassengleiche* maximal subgroup of index 2. Its HM symbol is $P12_11$, and the twofold rotations $\boldsymbol{2}$ of the point group $\boldsymbol{2}$ are realized by screw rotations $\boldsymbol{2}_1$ in this subgroup because $(t_C\,\boldsymbol{2}_0)$ is a screw rotation with its screw axis running parallel to the $\mathbf{b}$ axis through the point $\frac{1}{4}, 0, 0$. There are in fact these two *k*-subgroups of $C121$ of index 2 which have the group $\mathcal{T}_i$ in common. In the subgroup table of $C121$ both are listed under the heading 'Loss of centring translations' because the conventional unit cell is retained while only the centring translations have disappeared. (Four additional *klassengleiche* maximal subgroups of $C121$ are found under the heading 'Enlarged unit cell'.)

The group $\mathcal{T}_i$ of type $P1$ is a non-maximal subgroup of $C121$ of index 4.

Definition 1.2.6.2.5. A *klassengleiche* or *k*-subgroup $\mathcal{H} < \mathcal{G}$ is called *isomorphic* or an *isomorphic subgroup* if it belongs to the same affine space-group type (isomorphism type) as $\mathcal{G}$. If a subgroup is not isomorphic, it is sometimes called *non-isomorphic*. □

Isomorphic subgroups are special *k*-subgroups. The importance of the distinction between *k*-subgroups in general and isomorphic subgroups in particular stems from the fact that the number of maximal non-isomorphic *k*-subgroups of any space group is finite, whereas the number of maximal isomorphic subgroups is always infinite, see Section 1.2.8.

Example 1.2.6.2.6.

Consider a space group $\mathcal{G}$ of type $P\overline{1}$ referred to a conventional coordinate system. The translation subgroup $\mathcal{T}(\mathcal{G})$ consists of all translations with translation vectors $\mathbf{t} = u\mathbf{a}+v\mathbf{b}+w\mathbf{c}$, where u, v and w run through all integer numbers. There is an inversion $\overline{\boldsymbol{1}}_0$ with the inversion point at the origin and also an infinite number of other inversions, generated by the combinations of $\overline{\boldsymbol{1}}_0$ with all translations of $\mathcal{T}(\mathcal{G})$.

We consider the subgroup $\mathcal{T}_g$ of all translations with an even coefficient u and arbitrary integers v and w as well as the coset decomposition $(\mathcal{G} : \mathcal{T}_g)$. Let t_a be the translation with the translation vector $\mathbf{a}$. There are four cosets: $\mathcal{T}_g$, $\mathcal{T}_g\, t_a$, $\mathcal{T}_g\,\overline{\boldsymbol{1}}_0$ and $\mathcal{T}_g(t_a\,\overline{\boldsymbol{1}}_0)$. The union $\mathcal{T}_g \cup (\mathcal{T}_g\, t_a)$ forms the *translationengleiche* maximal subgroup $\mathcal{T}(\mathcal{G})$ of index 2. The union $\mathcal{T}_g \cup (\mathcal{T}_g\,\overline{\boldsymbol{1}}_0)$ forms an isomorphic maximal subgroup of index 2, as does the

[9] German: *zellengleiche* means 'with the same cell'; *translationengleiche* means 'with the same translations'; *klassengleiche* means 'of the same (crystal) class'. Of the different German declension endings only the form with terminal *-e* is used in this volume. The terms *zellengleiche* and *klassengleiche* were introduced by Hermann (1929). The term *zellengleiche* was later replaced by *translationengleiche* because of possible misinterpretations. In this volume they are sometimes abbreviated as *t*-subgroups and *k*-subgroups.

union $\mathcal{T}_g \cup (\mathcal{T}_g\,(t_a\,\overline{\boldsymbol{1}}_0))$. There are thus two maximal isomorphic subgroups of index 2 which are obtained by doubling the a lattice parameter. There are altogether 14 isomorphic subgroups of index 2 for any space group of type $P\overline{1}$ which are obtained by seven different cell enlargements.

If $\mathcal{G}$ belongs to a pair of enantiomorphic space-group types, then the isomorphic subgroups of $\mathcal{G}$ may belong to different crystallographic space-group types with different HM symbols and different space-group numbers. In this case, an infinite number of subgroups belong to the crystallographic space-group type of $\mathcal{G}$ and another infinite number belong to the enantiomorphic space-group type.

Example 1.2.6.2.7.

Space group $P4_1$, No. 76, has for any prime number $p > 2$ an isomorphic maximal subgroup of index p with the lattice parameters $a,\ b,\ pc$. This is an infinite number of subgroups because there is an infinite number of primes. The subgroups belong to the space-group type $P4_1$ if $p \equiv 1$ mod 4; they belong to the type $P4_3$ if $p \equiv 3$ mod 4.

Definition 1.2.6.2.8. A subgroup of a space group is called *general* or a *general subgroup* if it is neither a *translationengleiche* nor a *klassengleiche* subgroup. It has lost translations as well as linear parts, *i.e.* point-group symmetry. □

Example 1.2.6.2.9.

The subgroup $\mathcal{T}_g$ in Example 1.2.6.2.6 has lost all inversions of the original space group $P\overline{1}$ as well as all translations with odd u. It is a general subgroup $P1$ of the space group $P\overline{1}$ of index 4.

1.2.6.3. *The role of normalizers for group–subgroup pairs of space groups*

In Section 1.2.4.5, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of a subgroup $\mathcal{H} < \mathcal{G}$ in the group $\mathcal{G}$ was defined. The equation $\mathcal{H} \trianglelefteq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$ holds, *i.e.* $\mathcal{H}$ is a normal subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$, by its index in $\mathcal{G}$, determines the number $N_j = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$ of subgroups $\mathcal{H}_j < \mathcal{G}$ that are conjugate in the group $\mathcal{G}$, *cf.* Remarks (2) and (3) below Definition 1.2.4.5.1.

The group–subgroup relations between space groups become more transparent if one looks at them from a more general point of view. Space groups are part of the general theory of mappings. Particular groups are the *affine group* $\mathcal{A}$ of all reversible affine mappings, the *Euclidean group* $\mathcal{E}$ of all isometries, the *translation group* $\mathcal{T}$ of all translations and the *orthogonal group* $\mathcal{O}$ of all orthogonal mappings.

Connected with any particular space group $\mathcal{G}$ are its group of translations $\mathcal{T}(\mathcal{G})$ and its point group $\mathcal{P}_{\mathcal{G}}$. In addition, the normalizers $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of $\mathcal{G}$ in the affine group $\mathcal{A}$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ in the Euclidean group $\mathcal{E}$ are useful. They are listed in Section 15.2.1 of *IT* A. Although consisting of isometries only, $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is not necessarily a space group, see the paragraph below Lemma 1.2.7.2.6.

For the group–subgroup pairs $\mathcal{H} < \mathcal{G}$ the following relations hold:

(1) $\mathcal{T}(\mathcal{H}) \leq \mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G} \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G}) < \mathcal{E}$;

(1*a*) $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{H}) < \mathcal{E}$;

(1*b*) $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{A}}(\mathcal{H}) < \mathcal{A}$;

(2) $\mathcal{T}(\mathcal{H}) \leq \mathcal{T}(\mathcal{G}) < \mathcal{T} < \mathcal{E}$;

(3) $\mathcal{T}(\mathcal{G}) \leq \mathcal{G} \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{A}}(\mathcal{G}) < \mathcal{A}$.

The subgroup $\mathcal{H}$ may be a *translationengleiche* or a *klassengleiche* or a general subgroup of $\mathcal{G}$. In any case, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ determines the length of the conjugacy class of $\mathcal{H} < \mathcal{G}$, but it is not feasible to list for each group–subgroup pair $\mathcal{H} < \mathcal{G}$ its normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$. Indeed, it is only necessary to list for any space group $\mathcal{H}$ its normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ in the Euclidean group $\mathcal{E}$ of all isometries, as is done in *IT* A, Section 15.2.1. From such a list the normalizers for the group–subgroup pairs can be obtained easily, because for any chain of space groups $\mathcal{H} < \mathcal{G} < \mathcal{E}$, the relations $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{G}$ and $\mathcal{H} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{H}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{H})$ hold. The normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ consists consequently of all those isometries of $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ that are also elements of $\mathcal{G}$, *i.e.* that belong to the intersection $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) \cap \mathcal{G}$, *cf.* the examples of Section 1.2.7.[10]

The isomorphism type of the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ may depend on the lattice parameters of the space group (*specialized* Euclidean normalizer). For example, if the lattice of the space group $P\overline{1}$ of a triclinic crystal is accidentally monoclinic at a certain temperature and pressure or for a certain composition in a continuous solid-solution series, then the Euclidean normalizer of this space group belongs to the space-group types $P2/m$ or $C2/m$, otherwise it belongs to $P\overline{1}$. Such a *specialized Euclidean normalizer* (here $P2/m$ or $C2/m$) may be distinguished from the *typical Euclidean normalizer* (here $P\overline{1}$), for which the lattice of $\mathcal{H}$ is not more symmetric than is required by the symmetry of $\mathcal{H}$. The specialized Euclidean normalizers were first listed in the 5th edition of *IT* A (2002), Section 15.2.1.

1.2.7. Application to domain structures

1.2.7.1. *Introductory remarks*

In this section, the group-theoretical aspects of domain (twin) formation (domain structure, transformation twin) from a homogeneous single crystal (phase **A**, parent phase) to a crystalline phase **B** (daughter phase, deformed phase) are discussed, where the space group $\mathcal{H}$ of phase **B** is a subgroup of the space group $\mathcal{G}$ of phase **A**, $\mathcal{H} < \mathcal{G}$. This happens, *e.g.*, in a displacive or order–disorder phase transition. In most cases phase **B**, the *domain structure*, is inhomogeneous, consisting of homogeneous regions which are called *domains*, defined below.

Only the basic group-theoretical relations are considered here. A deeper discussion of domain structures and their properties needs methods using representation theory, thermodynamic points of view (Landau theory), lattice dynamics and tensor properties of crystals. Such treatments are beyond the scope of this section. A detailed discussion of them is given by Tolédano *et al.* (2003) and by Janovec & Přívratská (2003).

In order to make the group-theoretical treatment possible, the *parent-clamping approximation*, abbreviated PCA, is introduced, by which the lattice parameters of phase **A** are not allowed to change at and after the transition to phase **B**, *cf.* Janovec & Přívratská (2003). Under the assumption of the PCA, two essential conditions hold:

[10] For *maximal* subgroups, a calculation of the conjugacy classes is not necessary because these are indicated in the subgroup tables of Part 2 of this volume by braces to the left of the data sets for the low-index subgroups and by text for the series of isomorphic subgroups. For non-maximal subgroups, the conjugacy relations are not indicated but can be calculated in the way described here. They are also available online on the Bilbao crystallographic server, http://www.cryst.ehu.es/, under the program *Subgroupgraph*.

(1) The translations of phase **B** are translations of phase **A**. Thus, the space group $\mathcal{H}$ of **B** is a subgroup of the space group $\mathcal{G}$ of **A**, $\mathcal{H} < \mathcal{G}$. Without the PCA, the translations of **B** would not be translations of **A** and, therefore, **H** would not be a subgroup of **G**.

(2) Under the PCA, the more complicated ferroelastic phases[11] display the same simple behaviour as the non-ferroelastic ones. Disturbances which otherwise would be caused in ferroelastic phase transitions do not appear because there is no spontaneous strain.

The domain walls, *i.e.* the boundaries which separate different domains, will not be treated here because their symmetries are layer groups which are two-periodic groups in three-dimensional space and not space groups with three-dimensional periodicity. Layer groups are described in *International Tables for Crystallography*, Vol. E (2002).

Under these assumptions the domains formed may exhibit different chiralities and polarities of their structures and different spatial orientations of their symmetry elements, but each domain has the same specific energy and the lattice of each domain is part of the lattice of the parent structure **A** with space group $\mathcal{G}$.

In the discussion of domain structures, the following basic concepts are established: domain, domain state, symmetry state, orientation state. These concepts are defined and then applied in different examples of phase transitions in which the group-theoretical procedures and their results are explained.

The second step, the physically realistic situation at a temperature $T_x < T_C$ with the removal of the PCA, is only partly considered in this section. The relaxation of the PCA does not change the relations in a non-ferroelastic phase because all crystal regions suffer the same affine deformation. On the other hand, in ferroelastic phases the different spontaneous strains complicate the relations.

1.2.7.2. *Domains, domain states and symmetry states*

In a (continuous) phase transition with the symmetry reduction of the space group $\mathcal{G}$ to a subgroup $\mathcal{H} < \mathcal{G}$, a splitting of the parent phase **A** into many crystals of the type **B** is observed. The number of such crystals of **B** is not limited; they differ in their locations in space, in their orientations, in their shapes and in their space groups which, however, all belong to the same space-group type. In order to describe what happens in such a transition, a few notions are useful. If not explicitly stated, the validity of the PCA is assumed.

Definition 1.2.7.2.1. A connected homogeneous part of a domain structure or of a twinned crystal with structure type **B** is called a *domain*. Each domain is a single crystal. The part of the space that is occupied by a domain is the *region* of that domain. □

If the domains of phase **B** have been formed from a single crystal of phase **A**, then relations between the domains exist which are determined by group theory. In particular, the domains belong to a finite (small) number of domain states which have well defined relations to the original crystal **A** and its space group $\mathcal{G}$. In order to describe the relation of **B** to **A**, the notion of crystal pattern is used. Any perfect (ideal) crystal is a finite block of the corresponding infinite arrangement, the symmetry of which is a space group which contains translations. Here, this (infinite) periodic object is called a *crystal pattern*, *cf.* Section 1.2.2.1.

Definition 1.2.7.2.2. Two domains belong to the same *domain state* if their crystal patterns are identical, *i.e.* if they occupy different regions of space that are part of the *same* crystal pattern. In other words: a domain state is a crystal pattern. □

The number of domain states which are observed after a phase transition is limited and determined by the space groups $\mathcal{G}$ and $\mathcal{H}$. The number of domains which belong to the same domain state is not limited. The diversity of the domains and their shapes is due to mechanical stresses, defects, electrical charges and nucleation phenomena which strongly influence the kinetics of the phase transition.

A trivial domain structure is formed when phase **B** consists of one domain only, *i.e.* when it forms a *single-domain structure*. This is possible, in particular under an external electric field or under external stress. Such a procedure is known as 'detwinning'. The corresponding domain state is a *single-domain state*. For a phase transition of the type considered, there are always several single-domain states which have the same *a priori* probability of appearing after a phase transition. In reality not all of them will be observed and/or their relative frequencies and sizes will be rather different.

Single-domain states are introduced in theoretical considerations in order to avoid the complications which may be caused by the coexistence of domains with different spontaneous strain in ferroelastic crystals of the structure **B** if the PCA cannot be assumed. In polydomain structures, the domains would distort or rotate each other a little and thus disturb the simple relations described now. These disturbances do not occur in non-ferroelastic transitions, so for them the simple relations also hold in polydomain structures without the PCA.

Lemma 1.2.7.2.3. The number Z of possible domain states after a phase transition under the PCA is equal to the index i of $\mathcal{H}$ in $\mathcal{G}$, $Z = |\mathcal{G} : \mathcal{H}| = [i]$. Let $\mathcal{G} = \mathcal{H}_1 \cup \ldots \cup g_j\mathcal{H}_1 \cup \ldots \cup g_i\mathcal{H}_1$ be the coset decomposition of $\mathcal{G}$ relative to $\mathcal{H}_1$, where $g_1 = e, \ldots, g_i$ are the coset representatives, and $\mathcal{H}_1$ is the space group of the domain state $\mathbf{B}_1$. The other domain states are obtained from $\mathbf{B}_1$ by $\mathbf{B}_k = g_k\mathbf{B}_1$, $k = 2, \ldots, i$. For the space group $\mathcal{H}_k$ of the domain state $\mathbf{B}_k$ the following holds: $\mathcal{H}_k$ is obtained by conjugation of the space group $\mathcal{H}_1$ of $\mathbf{B}_1$ with the same element g_k: $\mathcal{H}_k = g_k\mathcal{H}_1g_k^{-1}$. □

If in a group–subgroup relation $\mathcal{G} > \mathcal{H}_q$ with index i_q the subgroups $\mathcal{H}_q$ belong to more than one conjugacy class, then each conjugacy class corresponds to a separate phase transition $\mathbf{A} \longrightarrow \mathbf{B}_k^{(1)}$, $\mathbf{A} \longrightarrow \mathbf{B}_k^{(2)}$ *etc*. These different phase transitions lead to different low-symmetry structures $\mathbf{B}^{(m)}$, have different transition temperatures and different probabilities of happening.

There are more elements of the group $\mathcal{G}$ than just g_k that map the domain state $\mathbf{B}_1$ onto the domain state $\mathbf{B}_k$. The elements of the space group $\mathcal{H}_1$ map the domain state of $\mathbf{B}_1$ onto itself: $h_m\mathbf{B}_1 = \mathbf{B}_1$, $h_m \in \mathcal{H}_1$. Therefore, not just the element g_k but all elements g_kh_m of the coset $g_k\mathcal{H}_1$ map the domain state of $\mathbf{B}_1$ onto the domain state $\mathbf{B}_k$: $\mathbf{B}_k = g_k\mathcal{H}_1\mathbf{B}_1 = g_k\mathbf{B}_1$. This can be expressed in the form:

There is a one-to-one correspondence between the cosets of the decomposition $(\mathcal{G} : \mathcal{H}_1)$ and the possible domain states which may be observed after the transition.

[11] A phase transition is called non-ferroelastic if the space groups $\mathcal{G}$ and $\mathcal{H}$ belong to the same crystal family, of which there are six: triclinic, monoclinic, orthorhombic, tetragonal, trigonal–hexagonal and cubic. A phase transition is called ferroelastic if the strain tensor of the low-symmetry phase **B** has more independent components than the strain tensor of the high-symmetry phase **A**. This can only happen if the space groups $\mathcal{G}$ of **A** and $\mathcal{H}$ of **B** belong to different crystal families. In this case, the additional components of the strain tensor of **B** are called *spontaneous strain-tensor components* or *components of the spontaneous deformation*.

Similarly, all elements $g_k h_m$ map the space group $\mathcal{H}_1$ onto $\mathcal{H}_k$ by conjugation: $\mathcal{H}_k = g_k h_m \mathcal{H}_1 h_m^{-1} g_k^{-1} = g_k \mathcal{H}_1 g_k^{-1}$.

Note that due to these formulae the *i* different domain states do not necessarily belong to *i* different space groups and that *different* domain states may belong to the *same* space group, *cf.* Lemma 1.2.7.2.6 and Example 1.2.7.2.4.

The terms just defined shall be explained in a few examples. By Example 1.2.7.2.4 a *translationengleiche* transition is displayed; *i.e.* $\mathcal{H}$ is a *translationengleiche* subgroup of $\mathcal{G}$. Then the relation between $\mathcal{G}$ and $\mathcal{H}$ is essentially reflected by the relation between the point groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}_{\mathcal{H}}$.

Example 1.2.7.2.4.

Perovskite $BaTiO_3$ exhibits a ferroelastic and ferroelectric phase transition from cubic to tetragonal, phase **A** with space group $\mathcal{G} = Pm\overline{3}m$, No. 221, and phase $\mathbf{B}_1$ with a *translationengleiche* subgroup $\mathcal{H}_1 = P4mm$, No. 99. Because the index $|\mathcal{G} : \mathcal{H}_1| = 6$, there are six domain states, forming three pairs of domain states which point with their tetragonal *c* axes along the cubic *x*, *y* and *z* axes of $\mathcal{G}$. Each pair consists of two antiparallel domain states of opposite polarization (ferroelectric domains). These two domain states belong to the same space group of the type *P*4*mm*, *i.e.* the domains of each pair belong to the same symmetry state according to the following definition:

Definition 1.2.7.2.5. Two domains belong to the same *symmetry state* if their space groups are identical. □

Note that here as in many other places of this section one has to distinguish strictly between 'space group' as a specimen, *e.g.* in 'space group of a crystal', and 'space-group type', which is one of the 230 classes frequently called simply but inexactly 'the 230 space groups', see the last paragraph of Section 1.2.5.3.

Domains of the same domain state always belong to the same symmetry state. Domains of different domain states may or may not belong to the same symmetry state. The number of symmetry states is limited and is smaller than or equal to the number of domain states. Moreover, the number of symmetry states is determined by the space groups $\mathcal{G}$ and $\mathcal{H}$.

Let $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ be the normalizer of the space group $\mathcal{H}_1$ in the space group $\mathcal{G}$. Then $\mathcal{G} \geq \mathcal{N}_{\mathcal{G}}(\mathcal{H}_1) \trianglerighteq \mathcal{H}_1$ with the indices $|\mathcal{G} : \mathcal{H}_1| = [i]$ and $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)| = [i_N]$ with $i_N \leq i$. By Lemma 1.2.7.2.3, the number $[i] = |\mathcal{G} : \mathcal{H}_1|$ of domain states is determined. For the number of symmetry states the following lemma holds:

Lemma 1.2.7.2.6. The number of symmetry states for the transition $\mathbf{A} \longrightarrow \mathbf{B}$ with space groups $\mathcal{G}$ and $\mathcal{H}$ is $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})| = i_N \leq i$. To each symmetry state there belong $d_i = i : i_N$ domain states, *i.e.* $d_i \cdot i_N = i$, *cf.* Janovec & Přívratská (2003). □

For the perovskite transition of Example 1.2.7.2.4, the normalizer $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ can be obtained from the Euclidean normalizer of *P*4*mm* in Table 15.2.1.4 of *IT* A which is listed as $P^1 4/mmm$. This Euclidean normalizer has continuous translations along the *z* direction (indicated by the P^1 lattice part of the HM symbol) and is thus not a space group. However, all additional translations of $P^1 4/mmm$ are not elements of the space group $\mathcal{G}$, and $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1) = (\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1) \cap \mathcal{G}) = (P^1 4/mmm \cap Pm\overline{3}m) = P4/mmm$ is a subgroup of $Pm\overline{3}m$ with index 3 and with the lattice of $Pm\overline{3}m$. Because of the index 3 of $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ in $\mathcal{G}$, there are three conjugate subgroups of the type *P*4*mm* with their fourfold axes directed along the *z*, *x* and *y* directions of the cubic space group $\mathcal{G}$. The group $\mathcal{H}_1$ is a subgroup of index 2 of $\mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$. Therefore, two domain states (with opposite polar axes) belong to each of the subgroups $\mathcal{H}_j$ of the space-group type *P*4*mm*.

In reality, *i.e.* without the PCA, the additional degree of freedom c/a in tetragonal space groups leads to a metrical inequivalence of the directions of the fourfold axis and the axes perpendicular to it, due to the spontaneous strain. If this 'true physical situation' is considered, the 90° angles between the fourfold axes of the domains of different pairs will change slightly because of the ferroelastic tetragonal deformation with subsequent small rotations of the domains. The antiparallel nature of each of the three domain pairs, however, is preserved because they exhibit the same symmetry state, *i.e.* belong to the same space group.

The space groups $\mathcal{G}$ and $\mathcal{H}$ in the phase transition in perovskites, *cf.* Example 1.2.7.2.4, are *translationengleiche*. Therefore, $\mathcal{T}(\mathcal{G}) = \mathcal{T}(\mathcal{H})$, and the coset decomposition $(\mathcal{G} : \mathcal{H})$ of the space groups corresponds to the coset decomposition $(\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}})$ of their point groups, *cf.* Section 1.2.6.2. Indeed, in the literature the perovskite transition is nearly always treated using point groups. Other than the *microscopic description* by space groups, the description by point groups is called the *macroscopic* or *continuum description*. Because there are no translations involved, the continuum approach does not require the PCA at all; the point group 4*mm* is for any translations of phase **B** a subgroup of the point group $m\overline{3}m$. However, the spontaneous strains will appear in this ferroelastic transition and will cause the complications mentioned at the end of Section 1.2.7.1 and in the paragraph preceding Lemma 1.2.7.2.3. For non-ferroelastic *translationengleiche* transitions, the application of point groups and of space groups yields equivalent results.

Example 1.2.7.2.4 presents an opportunity to mention another feature of this phase transition which, however, will not be discussed further. The group $\mathcal{H}_1$ is not a maximal subgroup of $\mathcal{G}$ but $\mathcal{G} > \mathcal{Z}_1 > \mathcal{H}_1$ with $\mathcal{Z}_1 = P4/mmm$ of index 3 in $\mathcal{G} = m\overline{3}m$ and $\mathcal{H}_1$ of index 2 in $\mathcal{Z}_1$. Such 'intermediate' domain states between **A** and **B**, like the domain state with the space group $\mathcal{Z}_1$, are called *secondary domain states* for thermodynamic reasons. They do not appear in the transition but $\mathcal{Z}_1$ is the symmetry of the spontaneous strain in the domain state with space group $\mathcal{H}_1$. Accidentally, in the present example $\mathcal{Z}_1 = \mathcal{N}_{\mathcal{G}}(\mathcal{H}_1)$ holds. Secondary domain states are treated by Janovec & Přívratská (2003).

1.2.7.3. *Translational domain structures (translation twins)*

In Example 1.2.7.2.4, a phase transition was discussed which involves only *translationengleiche* group–subgroup relations and, hence, only orientational relations between the domains. The following two examples treat *klassengleiche* transitions, *i.e.* $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{G}$, and *translational domain structures*, also called *translation twins*, may appear.

Translational domain structures consist of domains which are parallel, *i.e.* have the same orientation of their structures (and thus of their lattices) but differ in their location because of the loss of translations of the parent phase in the phase transition. The origins of the larger unit cells of the phase **B** with subgroup $\mathcal{H}$ may coincide with any of the origins of the smaller unit cells of the parent structure **A** with space group $\mathcal{G}$. Again the number of such domain states is equal to the index of $\mathcal{H}$ in $\mathcal{G}$, $[i] = |\mathcal{G} : \mathcal{H}|$; the number of symmetry states is $[i_N] = |\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})|$.

Example 1.2.7.3.1.

Let $\mathcal{G} = Fm\overline{3}m$, No. 225, with lattice parameter *a* and $\mathcal{H} = Pm\overline{3}m$, No. 221, with the same lattice parameter *a*. The relation $\mathcal{H} < \mathcal{G}$ is of index 4 and is found between the disordered and ordered modifications of the alloy $AuCu_3$. In the disordered state, one Au and three Cu atoms occupy the positions of a cubic F-lattice statistically; in the ordered compound the Au atoms occupy the positions of a cubic P-lattice whereas the Cu atoms occupy the centres of all faces of this cube. According to *IT* A, Table 15.2.1.4, the Euclidean normalizer of $\mathcal{H}$ is $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) = Im\overline{3}m$ with lattice parameter a. The additional I centring translations of $\mathcal{N}_{\mathcal{E}}(\mathcal{H})$ are not translations of $\mathcal{G}$ and thus $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = \mathcal{H}$. There are four domain states, each one with its own distinct space group and symmetry state $\mathcal{H}_j,\ j = 1, \ldots 4$, and consequently its own conventional origin relative to the origin of the disordered crystal **A** with the space group $\mathcal{G}$. The origin shifts of $\mathbf{B}_j$ relative to the origin of **A** are $0, 0, 0;\ \frac{1}{2}, \frac{1}{2}, 0;\ \frac{1}{2}, 0, \frac{1}{2}$ and $0, \frac{1}{2}, \frac{1}{2}$.

These shifts do not show up in the macroscopic properties of the domains. Indeed, one is normally neither interested in those translations of $\mathcal{G}$ which are lost in the transition to the subgroup $\mathcal{H}$, nor in the position of the conventional origin of **B** relative to that of **A** but only in the orientation of the domain states $\mathbf{B}_k$. If so, the observed relations are not governed by the space groups $\mathcal{G}$ and $\mathcal{H}$ but by $\mathcal{G}$ and *Hermann's group* $\mathcal{M}$, $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, *cf.* Lemma 1.2.8.1.2. The group $\mathcal{M}$ is uniquely determined as the space group with the translations of $\mathcal{G}$ and the point-group operations of $\mathcal{H}$. The group $\mathcal{M}$ can thus be characterized as that *translationengleiche* subgroup of $\mathcal{G}$ which is at the same time a *klassengleiche* supergroup of $\mathcal{H}$. This group $\mathcal{M}$ plays a role in the practical treatment of domains. It was applied to domain structures first by Janovec (1976).

In the current literature, the following considerations are mostly restricted to the point groups of the phases involved. In the following, the use of Hermann's group $\mathcal{M}$ is discussed in parallel with the normal use of the point groups. The (admittedly rather abstract) discussion may thus be unfamiliar to the reader. Nevertheless, it is offered here because it opens up the possibility of treating phase transitions on a microscopic or atomistic level, whereas the point-group approach can only deal with the continuum or macroscopic aspect. The microscopic approach is necessary in particular when discussing domain boundaries, which will not be done here.

Definition 1.2.7.3.2. Two domain states $\mathbf{B}_1$ and $\mathbf{B}_k$ with space groups $\mathcal{H}_1$ and $\mathcal{H}_k$ and point groups $\mathcal{P}_{\mathcal{H}_1}$ and $\mathcal{P}_{\mathcal{H}_k}$ have the *same orientation state* if their orientation is identical, *i.e.* if the linear part of the operation $g_k \in \mathcal{G}$ of Lemma 1.2.7.2.3 is the identity operation. This means that $g_k \in \mathcal{G}$ is a translation $t \in \mathcal{T}$ and implies that the point groups of $\mathbf{B}_1$ and $\mathbf{B}_k$ are the same: $\mathcal{P}_{\mathcal{H}_1} = \mathcal{P}_{\mathcal{H}_k}$. Thus the space groups $\mathcal{H}_1$ and $\mathcal{H}_k$ are subgroups of the same space group $\mathcal{M}$. □

Lemma 1.2.7.3.3. The number of orientation states in the transition $\mathbf{A} \longrightarrow \mathbf{B}$ with space groups $\mathcal{G} \longrightarrow \mathcal{H}_m$ is $|\mathcal{G} : \mathcal{M}_m|$, *i.e.* the index of $\mathcal{M}_m$ in $\mathcal{G}$, where $\mathcal{M}_m$ is Hermann's group in the sequence $\mathcal{G} \geq \mathcal{M}_m \geq \mathcal{H}_m$. These orientation states belong to $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{M}_m)|$ space groups. The number of domain states which belong to the same orientation state is $|\mathcal{M}_m : \mathcal{H}_m|$, *i.e.* the index of $\mathcal{H}_m$ in $\mathcal{M}_m$. □

In Example 1.2.7.3.1 of $AuCu_3$, $\mathcal{G} = \mathcal{M}_1$ because $\mathcal{H}_1$ is a *klassengleiche* subgroup of $\mathcal{G}$. Therefore, $|\mathcal{G} : \mathcal{M}_1| = 1$ and all four domain states belong to the same orientation state. This is obvious visually, because, as stated above, all four domain states are parallel and only shifted against each other.

Lemma 1.2.7.3.4. Because of the isomorphism $(\mathcal{G} : \mathcal{M}) \cong (\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}})$ between the factor groups $(\mathcal{G} : \mathcal{M})$ and $(\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}})$, the results of the application of the groups $\mathcal{G}$ and $\mathcal{M}$ are the same as the results of the application of the groups $\mathcal{P}_{\mathcal{G}}$ and $\mathcal{P}_{\mathcal{H}}$. The latter application is called the 'continuum approach to phase transitions' which is nearly always applied in practice. □

Lemma 1.2.7.3.3 is the microscopic formulation of the (macroscopic) continuum treatment of phase transitions and forms the bridge from the (macroscopic) continuum to the (microscopic) atomistic approach to phase transitions.

Example 1.2.7.3.5.

There is an order–disorder transition of the alloy β-brass, CuZn. In the disordered state the Cu and Zn atoms occupy statistically the positions of a cubic I lattice with space group $\mathcal{G} = Im\overline{3}m$, No. 229. In the ordered state, both kinds of atoms form a cubic primitive lattice P each, and one kind of atom occupies the centres of the cubes of the other, such that a space group $Pm\overline{3}m$, No. 221, is formed, see also Example 1.3.3.1. For the space groups the relation $\mathcal{G} = Im\overline{3}m > \mathcal{H} = Pm\overline{3}m$ of index 2 holds with the same cubic lattice parameter a. In this case, $\mathcal{G} = \mathcal{N}_{\mathcal{E}}(\mathcal{H})$, see *IT* A, Table 15.2.1.4. As the index $|\mathcal{G} : \mathcal{H}| = 2$, there are two domain states with their crystal structures shifted relative to each other by $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$. Thus, both domain states belong to the same orientation state. This also follows from $\mathcal{G} = \mathcal{M}$. Because $\mathcal{G} = \mathcal{N}_{\mathcal{G}}(\mathcal{H})$ and thus $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(\mathcal{H})| = 1$, there is one symmetry state, and both domain states belong to the same space group.

1.2.7.4. *Domain structures of a general phase transition*

Up to now, the examples have been concerned either with *translationengleiche* or with *klassengleiche* transitions only. In this section, the domain structure of a *general* transition will be considered, *i.e.* a transition where $\mathcal{H}$ is a general subgroup of $\mathcal{G}$. General subgroups are not listed in this volume but have to be derived from the maximal subgroups of each single step of the group–subgroup chain between $\mathcal{G}$ and $\mathcal{H}$. In the following Example 1.2.7.4.2, the chain has two steps. The results obtained under the PCA and without it are different and, therefore, will be discussed in some detail. Example 1.2.7.4.2 further shows how the subgroup data of this volume can be used for the analysis of continuous or quasi-continuous phase transitions.

We start with a lemma for general subgroups which contains the results of Lemmata 1.2.7.3.3 and 1.2.7.3.4.

Lemma 1.2.7.4.1. For general subgroups, owing to the existence of the group $\mathcal{M}$ of Hermann, it always holds that $|\mathcal{G} : \mathcal{H}| = |\mathcal{G} : \mathcal{M}| \cdot |\mathcal{M} : \mathcal{H}| = |\mathcal{P}_{\mathcal{G}} : \mathcal{P}_{\mathcal{H}}| \cdot |\mathcal{T}(\mathcal{G}) : \mathcal{T}(\mathcal{H})| = i_P \cdot i_T$. Here i_P is the index of the point groups of $\mathcal{G}$ and $\mathcal{H}$ and i_T is the index of the translation subgroups of $\mathcal{G}$ and $\mathcal{H}$. □

Example 1.2.7.4.2.

β-Gadolinium molybdate, $Gd_2(MoO_4)_3$, is ferroelectric and ferroelastic. The high-temperature phase **A** has space group $\mathcal{G} = P\overline{4}2_1m$, No. 113, and basis vectors **a**, **b** and **c**. At $T_C \sim 433$ K, a phase transition to a low-temperature phase **B** occurs with space-group type $\mathcal{H} = Pba2$, No. 32, basis vectors $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$ and $\mathbf{c}' = \mathbf{c}$. The group $\mathcal{M}$, $\mathcal{G} > \mathcal{M} > \mathcal{H}$ is of the type $Cmm2$ with the lattice parameters of $\mathcal{H}$. The index of $\mathcal{H}$ in $\mathcal{G}$ is $i = |P\overline{4}2_1m : Pba2| = 4$. A factor of 2 stems from the reduction $i_P = |\mathcal{G} : \mathcal{M}| = 2$ and leads to two orientation states. The other factor of 2 is caused by the loss of half of the translations, because $i_T = |\mathcal{M} : \mathcal{H}| = 2$.

In the continuum description, we consider the point groups and $|\overline{4}2m : mm2| = 2$. There is only one subgroup of $\overline{4}2m$ of the type $mm2$. Thus, the two orientation states belong to the same point group. The orientation state $\mathbf{B}_2$ is obtained from $\mathbf{B}_1$ by the (lost) $\overline{4}$ operation of $\overline{4}2m$.

This is the *macroscopic* or *continuum treatment*; it is the most common treatment of domains in phase transitions. In reality, *i.e.* lifting the PCA, due to the orthorhombic symmetry of phase **B** the domains will be slightly distorted and rotated, and thus the symmetry planes of the two domain states are no longer parallel.

The full microscopic or atomistic treatment has to consider the crystal structures of phases **A** and **B**. Under the PCA, the length of a' and b' is $(2)^{1/2}a$, the content of the unit cell of $\mathbf{B}_1$ is twice that of **A**. Because the index $[\,i\,] = 4$ there are four domain states $\mathbf{B}_1$ to $\mathbf{B}_4$ of $Pba2$. The domain state $\mathbf{B}_2$ is obtained from $\mathbf{B}_1$ by the (lost) $\overline{4}$ operation of $P\overline{4}2_1m$. The same holds for the pair $\mathbf{B}_3$ and $\mathbf{B}_4$. Thus, $\mathbf{B}_2$ & $\mathbf{B}_4$ are rotated by 90° around a $\overline{4}$ centre in the $(a'\,b')$ plane with respect to the pair $\mathbf{B}_1$ & $\mathbf{B}_3$, and the c' axes are antiparallel for $\mathbf{B}_2$ & $\mathbf{B}_4$ relative to those of $\mathbf{B}_1$ & $\mathbf{B}_3$. The orientation state of the pair $\mathbf{B}_1$ & $\mathbf{B}_3$ is different from that of $\mathbf{B}_2$ & $\mathbf{B}_4$. The two pairs $\mathbf{B}_1$ & $\mathbf{B}_2$ and $\mathbf{B}_3$ & $\mathbf{B}_4$ are shifted relative to each other by a (lost) translation of $P\overline{4}2_1m$, *e.g.* by $t(1,0,0)$ in the basis of $P\overline{4}2_1m$, corresponding to $t(\frac{1}{2},\frac{1}{2},0)$ in the basis of $Pba2$.

To calculate the number of space groups $Pba2$, *i.e.* the number of symmetry states, one determines the normalizer of $Pba2$ in $P\overline{4}2_1m$. From *IT* A, Table 15.2.1.3, one finds $\mathcal{N}_{\mathcal{E}}(Pba2) = P^14/mmm$ for the Euclidean normalizer of $Pba2$ under the PCA, which includes the condition $a = b$. P^14/mmm is a supergroup of $P\overline{4}2_1m$. Thus, $\mathcal{N}_{\mathcal{G}}(Pba2) = (\mathcal{N}_{\mathcal{E}}(Pba2) \cap \mathcal{G}) = \mathcal{G}$ and $|\mathcal{G} : \mathcal{N}_{\mathcal{G}}(Pba2)| = |\mathcal{G} : \mathcal{G}| = 1$. Therefore, under the PCA all four domain states belong to one symmetry state, *i.e.* to one space group $Pba2$.

Analysing the group–subgroup relations between $P\overline{4}2_1m$ and $Pba2$ with the tables of this volume, one finds only one chain $P\overline{4}2_1m \rightarrow Cmm2 \rightarrow Pba2$. For $P\overline{4}2_1m$ only one maximal subgroup of type $Cmm2$ is listed, for which again only one maximal subgroup of type $Pba2$ is found, in agreement with the previous paragraph.

In reality, *i.e.* relaxing the PCA, the observations are made at temperatures $T_x < T_C$ where the lattice parameters deviate from those of phase **A** and the basis no longer has tetragonal symmetry, but orthorhombic symmetry, $a' < b'$. The previous single space group now splits into *two* different space groups of type $Pba2$ with orthorhombic metrics at T_x, one belonging to the pair $\mathbf{B}_1$ & $\mathbf{B}_3$, the other to $\mathbf{B}_2$ & $\mathbf{B}_4$. The $(\mathbf{a}', \mathbf{b}')$ bases of these pairs are oriented perpendicular to each other and the $\mathbf{c}'$ axes of their domains are antiparallel. The loss of the centring translation of $Cmm2$ does not produce a new space group.

The number, two, of these space groups if the PCA is not valid can also be calculated in the usual way with the help of the normalizer. The Euclidean normalizer of $Pba2$ with $a' \neq b'$ is $\mathcal{N}_{\mathcal{E}}(Pba2) = P^1mmm$. This is an orthorhombic group with continuous translations along the $\mathbf{c}'$ direction. P^1mmm with $a' \neq b'$ is not really a subgroup of $P\overline{4}2_1m$ because the translations of $Pba2$ and thus of $Cmm2$ and P^1mmm are not strictly translations of $P\overline{4}2_1m$. The first three groups have orthorhombic lattices and the last a tetragonal one. However, by relaxing the PCA only gradually, the difference between the orthorhombic groups and the corresponding groups with tetragonal lattices is arbitrarily small. Therefore, one considers the sequence $\mathcal{G} > \mathcal{M} = \mathcal{N}_{\mathcal{G}}(\mathcal{H}) > \mathcal{H}$, *i.e.* $P\overline{4}2_1m > Cmm2 > Pba2$ as a group–subgroup chain, forms the intersection $(P^1mmm \cap P\overline{4}2_1m)$ as if the groups would have common translations, and finds $\mathcal{N}_{\mathcal{G}}(\mathcal{H}) = Cmm2$ with approximately the lattice parameters of $P\overline{4}2_1m$. The index $|P\overline{4}2_1m : Cmm2| = 2$, such that there are two space groups of type $Pba2$ which are approximately subgroups of $P\overline{4}2_1m$. To each of these space groups $Pba2$ belong two domain states of phase **B**, see above.

This example shows that without the PCA, in order to cope with real observations, the terms 'subgroup', 'intersection of groups' *etc.* must not be used *sensu stricto* but have to be relaxed. The orthorhombic translations in this example are not group elements of $\mathcal{G}$ but are slightly modified from the original translations of $\mathcal{G}$. All group–subgroup relations in crystal chemistry, *e.g.* diamond (C)–sphalerite (ZnS), as well as many phase transitions, as in this example, require such a 'softened' approach.

It turns out that the transition of $Gd_2(MoO_4)_3$ can be considered both under the PCA (allowing exact group-theoretical arguments) and under physically realistic arguments (which require certain relaxations of the group-theoretical methods). The results are different but the realistic approach can be developed by means of an increasing deviation from the PCA, starting from idealized but unrealistic considerations.

1.2.8. Lemmata on subgroups of space groups

There are several lemmata on subgroups $\mathcal{H} < \mathcal{G}$ of space groups $\mathcal{G}$ which may help in getting an insight into the laws governing group–subgroup relations of plane and space groups. They were also used for the derivation and the checking of the tables of Part 2. These lemmata are proved or at least stated and explained in Chapter 1.5. They are repeated here as statements, separated from their mathematical background, and are formulated for the three-dimensional space groups. They are valid by analogy for the (two-dimensional) plane groups.

1.2.8.1. *General lemmata*

Lemma 1.2.8.1.1. A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is a space group again, if and only if the index $i = |\mathcal{G} : \mathcal{H}|$ is finite. □

In this volume, only subgroups of finite index i are listed. However, the index i is not restricted, *i.e.* there is no number I with the property $i < I$ for any i. Subgroups $\mathcal{H} < \mathcal{G}$ with infinite index are considered in *International Tables for Crystallography*, Vol. E (2002).

Lemma 1.2.8.1.2. Hermann's theorem. For any group–subgroup chain $\mathcal{G} > \mathcal{H}$ between space groups there exists a uniquely defined space group $\mathcal{M}$ with $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, where $\mathcal{M}$ is a *translationengleiche* subgroup of $\mathcal{G}$ and $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{M}$. □

The decisive point is that any group–subgroup chain between space groups can be split into a *translationengleiche* subgroup chain between the space groups $\mathcal{G}$ and $\mathcal{M}$ and a *klassengleiche* subgroup chain between the space groups $\mathcal{M}$ and $\mathcal{H}$.

It may happen that either $\mathcal{G} = \mathcal{M}$ or $\mathcal{H} = \mathcal{M}$ holds. In particular, one of these equations must hold if $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of $\mathcal{G}$.

Lemma 1.2.8.1.3. (Corollary to Hermann's theorem.) A maximal subgroup of a space group is either a *translationengleiche* subgroup or a *klassengleiche* subgroup, never a general subgroup. □

The following lemma holds for space groups but not for arbitrary groups of infinite order.

Lemma 1.2.8.1.4. For any space group, the number of subgroups with a given finite index i is *finite*. □

This number of subgroups can be further specified, see Chapter 1.5. Although for each index i the number of subgroups is finite, the number of all subgroups with finite index is infinite because there is no upper limit for the number i.

1.2.8.2. *Lemmata on maximal subgroups*

Even the set of all *maximal* subgroups of finite index is not finite, as can be seen from the following lemma.

Lemma 1.2.8.2.1. The index i of a maximal subgroup of a space group is always of the form p^n, where p is a prime number and $n = 1$ or 2 for plane groups and $n = 1,\ 2$ or 3 for space groups. □

An index of $p^2,\ p > 2$, occurs only for isomorphic subgroups of tetragonal, trigonal and hexagonal space groups when the basis vectors are enlarged to $p\mathbf{a}$, $p\mathbf{b}$. An index of p^3 occurs for and only for isomorphic subgroups of cubic space groups with cell enlargements of $p\mathbf{a}$, $p\mathbf{b}$, $p\mathbf{c}$ $(p > 2)$.

This lemma means that a subgroup of, say, index 6 cannot be maximal. Moreover, because of the infinite number of primes, the set of all maximal subgroups of a given space group cannot be finite.

There are even stronger restrictions for *maximal non-isomorphic* subgroups.

Lemma 1.2.8.2.2. The index of a maximal non-isomorphic subgroup of a plane group is 2 or 3; for a space group the index is 2, 3 or 4. □

This lemma can be specified further:

Lemma 1.2.8.2.3. The index of a maximal non-isomorphic subgroup $\mathcal{H}$ is always 2 for oblique, rectangular and square plane groups and for triclinic, monoclinic, orthorhombic and tetragonal space groups $\mathcal{G}$. The index is 2 or 3 for hexagonal plane groups and for trigonal and hexagonal space groups $\mathcal{G}$. The index is 2, 3 or 4 for cubic space groups $\mathcal{G}$. □

There are also lemmata for the number of subgroups of a certain index. The most important are:

Lemma 1.2.8.2.4. The number of subgroups of index 2 is $2^N - 1$ with $0 \le N \le 6$ for space groups and $0 \le N \le 4$ for plane groups. The number of *translationengleiche* subgroups of index 2 is $2^M - 1$ with $0 \le M \le 3$ for space groups and $0 \le M \le 2$ for plane groups. □

Examples are:

$N = 0:\ 2^0 - 1 = 0$ subgroups of index 2 for $p3$, No. 13, and $F23$, No. 196;

$N = 1:\ 2^1 - 1 = 1$ subgroup of index 2 for $p3m1$, No. 14, and $P3$, No. 143; . . . ;

$N = 4:\ 2^4 - 1 = 15$ subgroups of index 2 for $p2mm$, No. 6, and $P\overline{1}$, No. 2;

$N = 6:\ 2^6 - 1 = 63$ subgroups of index 2 for $Pmmm$, No. 47.

Lemma 1.2.8.2.5. The number of isomorphic subgroups of each space group is infinite and this applies even to the number of maximal isomorphic subgroups. □

Nevertheless, their listing is possible in the form of infinite series. The series are specified by parameters.

Lemma 1.2.8.2.6. For each space group, each maximal isomorphic subgroup $\mathcal{H}$ can be listed as a member of one of at most four series of maximal isomorphic subgroups. Each member is specified by a set of parameters. □

The series of maximal isomorphic subgroups are discussed in Section 2.1.5.

references

1.3. Remarks on Wyckoff positions

By Ulrich Müller

1.3.1. Introduction

Symmetry relations using crystallographic group–subgroup relations have proved to be a valuable tool in crystal chemistry and crystal physics. Some important applications include :

(1) Structural relations between crystal-structure types can be worked out in a clear and concise manner by setting up family trees of group–subgroup relations (Bärnighausen, 1980; Baur, 1994; Baur & McLarnan, 1982; Bock & Müller, 2002*a*,*b*; Chapuis, 1992; Meyer, 1981; Müller, 1993, 2002; Pöttgen & Hoffmann, 2001).

(2) Elucidation of problems concerning twinned crystals and antiphase domains (*cf.* Section 1.2.7, p. 18; Bärnighausen, 1980; van Tendeloo & Amelinckx, 1974; Wondratschek & Jeitschko, 1976).

(3) Changes of structures and physical properties taking place during phase transitions: applications of Landau theory (Aroyo & Perez-Mato, 1998; Birman, 1966*a*,*b*; Cracknell, 1975; Izyumov & Syromyatnikov, 1990; Landau & Lifshitz, 1980; Salje, 1990; Stokes & Hatch, 1988; Tolédano & Tolédano, 1987).

(4) Prediction of crystal-structure types and calculation of the numbers of possible structure types (McLarnan, 1981*a*,*b*,*c*; Müller, 1978, 1980, 1981, 1986, 1992, 1998, 2003).

All of these applications require consideration of the relations between the atomic sites in a space group and in the corresponding subgroups.

1.3.2. Crystallographic orbits and Wyckoff positions

The set of symmetry-equivalent sites in a space group is referred to as a (*crystallographic point*) *orbit* (Koch & Fischer, 1985; Wondratschek, 1976, 1980, 2002; also called *point configuration*). If the coordinates of a site are completely fixed by symmetry (*e.g.* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$), then the orbit is identical with the corresponding *Wyckoff position* of that space group (in German *Punktlage*). However, if there are one or more freely variable coordinates (*e.g.* z in $0, \frac{1}{2}, z$), the Wyckoff position comprises an infinity of possible orbits; they differ in the values of the variable coordinate(s). The set of sites that are symmetry equivalent to, say, $0, \frac{1}{2}, 0.391$ make up one orbit. The set corresponding to $0, \frac{1}{2}, 0.468$ belongs to the same Wyckoff position, but to another orbit (its variable coordinate z is different).

The Wyckoff positions of the space groups are listed in Volume A of *International Tables for Crystallography* (2002). They are labelled with letters a, b, ..., beginning from the position having the highest site symmetry. A Wyckoff position is usually given together with the number of points belonging to one of its orbits within a unit cell. This number is the *multiplicity* listed in Volume A, and commonly is set in front of the Wyckoff letter. For example, the denomination $4c$ designates the four symmetry-equivalent points belonging to an orbit c within the unit cell.

In many space groups, for some Wyckoff positions there exist several Wyckoff positions of the same kind that can be combined to form a *Wyckoff set* [called a *Konfigurationslage* by Koch & Fischer (1975)]. They have the same site symmetries and they are mapped onto one another by the affine normalizer of the space group (Koch & Fischer, 1975; Wondratschek, 2002).

Example 1.3.2.1.

In space group $I222$, No. 23, there are six Wyckoff positions with the site symmetry 2:

$4e\ (x, 0, 0)$, $4f\ (x, 0, \frac{1}{2})$ on twofold rotation axes parallel to **a**,

$4g\ (0, y, 0)$, $4h\ (\frac{1}{2}, y, 0)$ on twofold rotation axes parallel to **b**,

$4i\ (0, 0, z)$, $4j\ (0, \frac{1}{2}, z)$ on twofold rotation axes parallel to **c**.

They are mapped onto one another by the affine normalizer of $I222$, which is isomorphic to $Pm\bar{3}m$, No. 221. These six Wyckoff positions make up one Wyckoff set.

However, in this example the positions $4e$, $4f$ *vs.* $4g$, $4h$ *vs.* $4i$, $4j$, being on differently oriented axes, cannot be considered to be equivalent if the lattice parameters are $a \neq b \neq c$. The subdivision of the positions of the Wyckoff set into these three sets is accomplished with the aid of the *Euclidean normalizer* of the space group $I222$.

The Euclidean normalizer is that supergroup of a space group that maps all equivalent symmetry elements onto one another without distortions of the lattice. It is a subgroup of the affine normalizer (Fischer & Koch, 1983; Koch *et al.*, 2002). In Example 1.3.2.1 (space group $I222$), the positions $4e$ and $4f$ are equivalent under the Euclidean normalizer (and so are $4g$, $4h$ and also $4i$, $4j$). The Euclidean normalizer of the space group $I222$ is $Pmmm$, No. 47, with the lattice parameters $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$ (if $a \neq b \neq c$). If the origin of a space group is shifted, Wyckoff positions that are equivalent under the Euclidean normalizer may have to be interchanged. The permutations they undergo when the origin is shifted have been listed by Boyle & Lawrenson (1973). An origin shift of $0, 0, \frac{1}{2}$ will interchange the Wyckoff positions $4e$ and $4f$ as well as $4g$ and $4h$ of $I222$.

Example 1.3.2.2.

In the space group $Fm\bar{3}m$, No. 225, the orbits of the Wyckoff positions $4a\ (0, 0, 0)$ and $4b\ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ are equivalent under the Euclidean normalizer. The copper structure can be described equivalently either by having the Cu atoms occupy the position $4a$ or the position $4b$. If we take Cu atoms in the position $4a$ and shift the origin from $(0, 0, 0)$ to $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, then they result in the position $4b$.

Unique relations exist between the Wyckoff positions of a space group and the Wyckoff positions of any of its subgroups (Billiet *et al.*, 1978; Wondratschek, 1993; Wondratschek *et al.*, 1995). Given the relative positions of their unit cells (axes transformations and relative origin positions), the labels of these Wyckoff positions are unique.

Example 1.3.2.3.

In diamond, the carbon atoms occupy the orbit belonging to the Wyckoff position $8a$ of the space group $Fd\bar{3}m$, No. 227. Sphalerite (zinc blende) crystallizes in the maximal subgroup $F\bar{4}3m$, No. 216, of $Fd\bar{3}m$. With the transition $Fd\bar{3}m \rightarrow F\bar{4}3m$ the Wyckoff position $8a$ splits into the positions $4a$ and $4c$ of $F\bar{4}3m$.

These are two symmetry-independent positions that allow an occupation by atoms of two different elements (zinc and sulfur). In this example, all of the positions retain the site symmetry $\overline{4}3m$ and each Wyckoff position comprises only one orbit.

1.3.3. Derivative structures and phase transitions

In crystal chemistry, structural relations such as the relation diamond–sphalerite are of fundamental interest. Structures that result from a *basis structure* by the substitution of atoms of one kind for atoms of different elements, the topology being retained, are called *derivative structures* after Buerger (1947, 1951). For the basis structure the term *aristotype* has also been coined, while its derivative structures are called *hettotypes* (Megaw, 1973). When searching for derivative structures, one must look for space groups that are subgroups of the space group of the aristotype *and* in which the orbit of the atom(s) to be substituted splits into different orbits.

Similar relations also apply to many phase transitions. Very often the space group of one of the phases is a subgroup of the space group of the other. For second-order phase transitions this is even mandatory (*cf.* Section 1.2.7). The positions of the atoms in one phase are related to those in the other one.

Example 1.3.3.1.

The disorder–order transition of β-brass (CuZn) taking place at 741 K involves a space-group change from the space group $Im\overline{3}m$, No. 229, to its subgroup $Pm\overline{3}m$, No. 221. In the high-temperature form, Cu and Zn atoms randomly take the orbit of the Wyckoff position $2a$ of $Im\overline{3}m$. Upon transition to the ordered form, this position splits into the independent positions $1a$ and $1b$ of the subgroup $Pm\overline{3}m$. These positions are occupied by the Cu and Zn atoms, respectively. See also Example 1.2.7.3.5.

Phase transitions in which a paraelectric crystal becomes ferroelectric occur when atoms that randomly occupy several symmetry-equivalent positions become ordered in a space group with lower symmetry, or when a key atom is displaced to a position with reduced site symmetry, thus allowing a distortion of the structure. In both cases, the space group of the ferroelectric phase is a subgroup of the space group of the paraelectric phase. In the case of ordering, the orbits of the atoms concerned split; in the case of displacement this is not necessary.

Example 1.3.3.2.

In paraelectric $NaNO_2$, space group $Immm$, No. 71, Na^+ ions randomly occupy two sites close to each other around an inversion centre $(0, 0, \frac{1}{2})$ with half occupation (position $4i$ at $0, 0, \pm 0.540$). The same applies to the nitrite ions, which are disordered in two opposite orientations around the inversion centre at 0, 0, 0, with the N atoms at $4i$ $(0, 0, \pm 0.072)$. At the transition to the ferroelectric phase at 438 K, the space-group symmetry decreases to the subgroup $Imm2$, No.44, and the ions become ordered in one orientation. Each of the $4i$ orbits splits into two $2a$ orbits, but for every ion only one of the resulting orbits is now fully occupied: Na^+ at $2a$ (0, 0, 0.540) and N at $2a$ (0, 0, 0.074).

Example 1.3.3.3.

Paraelectric $BaTiO_3$ crystallizes in the space group $Pm\overline{3}m$, No. 221, and the position $1a$ of a Ti atom (0, 0, 0 with site symmetry $m\overline{3}m$) is in the centre of an octahedron of oxygen atoms. At 393 K, a phase transition to a ferroelectric phase takes place. It has space group $P4mm$, No. 99, which is a subgroup of $Pm\overline{3}m$; the Ti atom is now at $0, 0, z$ ($1a$, site symmetry $4mm$) and is displaced from the octahedron centre. The orbit does not split, but the site symmetry is reduced.

1.3.4. Relations between the positions in group–subgroup relations

The following statements are universally valid:

(1) Between the points of an orbit and the corresponding points in a subgroup there exists a one-to-one relation; both sets of points have the same magnitude.

(2) Between the Wyckoff positions of a space group and those of its subgroups there exist unique relations. These may involve different Wyckoff labels for different relative positions of the origins.

(3) With the symmetry reduction from a group to a subgroup, an orbit either splits into different orbits, or its site symmetry is reduced, or both happen. In addition, coordinates fixed or coupled by symmetry may become independent.

Let $\mathcal{G}$ be a space group and $\mathcal{H}$ a subgroup of $\mathcal{G}$. Let the site-symmetry groups of a point X under the space groups $\mathcal{G}$ and $\mathcal{H}$ be $\mathcal{S}_{\mathcal{G}}(X)$ and $\mathcal{S}_{\mathcal{H}}(X)$, respectively. The reduction factor of the site symmetries is then

$$R_j = |\mathcal{S}_{\mathcal{G}}(X)|/|\mathcal{S}_{\mathcal{H}}(X)|.$$

When the space-group symmetry is reduced from $\mathcal{G}$ to $\mathcal{H}$ and the orbit of the point X splits into n orbits, the following relation holds (Wondratschek, 2002):

$$i = \sum_{j=1}^{n} R_j.$$

$i = |\mathcal{G} : \mathcal{H}|$ is the index of $\mathcal{H}$ in $\mathcal{G}$ (*cf.* Section 1.2.4.2).

Example 1.3.4.1.

The orbit of the Wyckoff position $24d$ of space group $Fm\overline{3}m$, No. 225, has the site symmetry mmm with the order $|mmm| = 8$. Upon symmetry reduction to the space group $I4/mmm$, No. 139, this orbit splits into the two orbits $4c$ and $8f$ of $I4/mmm$ with the site symmetries mmm and $2/m$, respectively. $|2/m| = 4$. The reduction factors of the site symmetries are

$$|mmm|/|mmm| = 8/8 = 1 \quad \text{and} \quad |mmm|/|2/m| = 8/4 = 2.$$

They add up to $1 + 2 = 3$, which is the index of $I4/mmm$ in $Fm\overline{3}m$.

The multiplicities commonly used together with the Wyckoff labels depend on the size of the chosen unit cell. As a consequence, a change of the size of the unit cell also changes the multiplicities. For example, the multiplicities of the Wyckoff positions listed in Volume A are larger by a factor of three for rhombohedral space groups when the unit cell is referred not to rhombohedral, but to hexagonal axes.

The multiplicity of a Wyckoff position shows up in the sum of the multiplicities of the corresponding positions of the subgroup. If the unit cell selected to describe the subgroup does not change in size, then the sum of the multiplicities of the positions of the subgroup must be equal to the multiplicity of the position of the starting group. For example, from a position with a multiplicity of 6, a position with multiplicity of 6 can result, or it can split into two positions of multiplicity of 3, or into two with multiplicities of 2 and 4, or into three with multiplicity of 2 *etc.* If the unit cell of the subgroup is enlarged or reduced by a factor f, then the sum of the multiplicities must also be multiplied or divided by this factor f.

Relations between the Wyckoff positions of space groups and the Wyckoff positions of their maximal subgroups were listed by Lawrenson (1972). However, his tables are not complete, and they were never published. In addition, they lack information about the transformations of axes and coordinates when these differ in the subgroup.

More recently, a computer program to calculate these relations has been developed (Kroumova *et al.*, 1998). To be used, the program requires knowledge of the subgroups (maximal or non-maximal) and of the necessary axes transformations and origin shifts. The Wyckoff position(s) to be considered can be marked or specific coordinates of a position must be given. The output is a listing of the Wyckoff position(s) of the specified subgroup and optionally all corresponding site coordinates. Depending on the relations and positions considered, the listings of coordinates can be rather long. The program has not been designed to give a fast overview of the relations. If one is looking for those subgroups that will exhibit a splitting of a certain position, all subgroups have to be tried one by one. For these reasons, the program cannot substitute the present tables; for practical work, the program and the tables listed in Part 3 complement each other.

The tables in Part 3 are a complete compilation for all space groups and all of their maximal subgroups. For all Wyckoff positions of a space group, all relations to the Wyckoff positions of its subgroups are listed. This also applies to the infinite number of maximal isomorphic subgroups; for these, a parameterized form has been developed that allows the listing of all maximal subgroups and all of their resulting Wyckoff positions completely for every allowed index of symmetry reduction.

references

International Tables for Crystallography (2006). Vol. A, Chapter 1.4, pp. 27–28.

1.4. Computer checking of the subgroup data

By Franz Gähler

1.4.1. Introduction

Most of the data in Part 2 of this volume have been checked by a computer-algebra program. This program is built upon the package *Cryst* (Eick *et al.*, 2001), formerly known as *CrystGAP* (Eick *et al.*, 1997), which in turn is an extension of the computer-algebra program *GAP* (The *GAP* Group, 2002). *GAP* is a program system for computations involving general algebraic structures, in particular groups. Since space groups are infinite groups, the generic algorithms for finite groups often cannot be used for space groups. The *Cryst* package provides the special methods and algorithms needed for working with space groups, thereby extending the field of applicability of *GAP*. The algorithms used in *Cryst* have been described by Eick *et al.* (1997).

1.4.2. Basic capabilities of the *Cryst* package

Before we describe in more detail the checks that have been performed, we briefly summarize the capabilities of the *Cryst* package and how space groups are handled by *Cryst*.

In *Cryst*, a space group is represented as a fixed group of augmented matrices $\mathbb{W}_i$, *cf.* Section 1.2.2.4. The group multiplication therefore coincides with matrix multiplication. The space group is defined by an arbitrary (finite) set of generating elements. The space group consists of the set of all augmented matrices that can be obtained as products of the generating matrices. It is not important which generating elements are chosen. Different sets of generators can define the same space group.

The representation of a space group as a group of augmented matrices implicitly requires the choice of an origin and a vector basis of Euclidean space. The *Cryst* package does not require any particular choice of origin or vector basis. In particular, it is not necessary to work with a lattice basis; in fact, any basis can be used. This has the advantage that one can continue to use the basis chosen for the parent group when passing to a subgroup.

Space groups are conjugated by some affine coordinate transformation if they differ only in their settings, *i.e.* by the choice of their origins and/or vector bases. Such an affine coordinate transformation is also represented by an augmented matrix. Given a coordinate transformation $\mathbb{V}$ and a space group $\mathcal{G}$, the transformed space group $\mathcal{G}'$ is simply generated by the transformed generators of $\mathcal{G}$.

If a space group $\mathcal{G}$ is given by a set of generators, *Cryst* first needs to compute the point group $\mathcal{P}$ of $\mathcal{G}$, and the translation subgroup $\mathcal{T}$, represented by a (canonical) basis of the translation lattice (the basis of the translation lattice chosen by *Cryst* is canonical in the sense that the same basis is always chosen for a given $\mathcal{T}$). The point group $\mathcal{P}$ is simply generated by the linear parts of the generators of $\mathcal{G}$. The mapping H, which sends each element of $\mathcal{G}$ to its linear part, is in fact a group homomorphism $\mathsf{H}\colon \mathcal{G} \longrightarrow \mathcal{P}$. The point group $\mathcal{P}$ is finite and each point-group element p can easily be expressed as a product of generators of $\mathcal{P}$, which are images of generators of $\mathcal{G}$ under H. This provides a way to compute, for any $p \in \mathcal{P}$, some representative pre-image g of p under H, *i.e.* some element $g \in \mathcal{G}$ which is mapped onto p by H. Having expressed the element p as a product of generators, one simply replaces the factors in this product by their representative pre-images under H, which are known by construction, to obtain the representative pre-image g of p.

To compute a generating set of the translation subgroup $\mathcal{T} \leq \mathcal{G}$, one first computes a set of defining relations of the point group $\mathcal{P}$ for the given generators. For a finite group this is a standard task in *GAP*. These defining relations are a set of inequivalent ways to express the identity element of $\mathcal{P}$ by the generators of $\mathcal{P}$. Replacing the factors in such a defining relation by their representative pre-images in $\mathcal{G}$ yields a pre-image of the identity of $\mathcal{P}$, *i.e.* an element of $\mathcal{T}$. The translations so obtained generate, together with the pure translation generators of $\mathcal{G}$, the entire translation subgroup $\mathcal{T} \leq \mathcal{G}$.

We now have all the necessary information to test whether a given augmented matrix $\mathbb{A}$ is an element of a space group $\mathcal{G}$. One first tests whether the linear part $\boldsymbol{M}$ of $\mathbb{A}$ is an element of the point group $\mathcal{P}$ of $\mathcal{G}$. If $\boldsymbol{M} \notin \mathcal{P}$, $\mathbb{A}$ is not an element of $\mathcal{G}$. Otherwise, some pre-image $\mathbb{G}$ of $\boldsymbol{M}$ in $\mathcal{G}$ is computed. $\mathbb{A}$ is then an element of $\mathcal{G}$ if and only if $\mathbb{A}$ and $\mathbb{G}$ differ in their translation part by an element of the translation group $\mathcal{T}$. With this membership test, we can determine whether two space groups are equal, or whether one is a subgroup of the other: a space group $\mathcal{H}$ is a subgroup of a space group $\mathcal{G}$ if all the generators of $\mathcal{H}$ are elements of $\mathcal{G}$. Two space groups are equal if either of them is a subgroup of index 1 of the other.

1.4.3. Computing maximal subgroups

The *Cryst* package has built-in facilities for computing the maximal subgroups of a given index for any space group $\mathcal{G}$. More precisely, given a prime number p, *Cryst* can compute conjugacy-class representatives of those maximal subgroups of $\mathcal{G}$ whose index in $\mathcal{G}$ is a power of p. The algorithms used for this task are described in Eick *et al.* (1997). Essentially, one determines the maximal subgroups of the (finite) factor group $\mathcal{G}/\mathcal{T}_p$, where $\mathcal{T}_p$ is the subgroup of those translations of $\mathcal{G}$ which are a p-fold multiple of an element of the full translation group $\mathcal{T}$ of $\mathcal{G}$. After the maximal subgroups are obtained, the translations in $\mathcal{T}_p$ are added back to the subgroups.

From a representative $\mathcal{H}$ of a conjugacy class of subgroups, the list of all subgroups in the same conjugacy class is obtained by repeatedly conjugating $\mathcal{H}$ (and the subgroups obtained from it by conjugation) with generators of $\mathcal{G}$, until no new conjugated subgroups are obtained. This is also the way of determining whether two subgroups are conjugated: one enumerates the groups in the conjugacy class of one of them, and checks whether the other is among them.

The index of a subgroup $\mathcal{H}$ of $\mathcal{G}$ is easily computed as the product of the index of the point group of $\mathcal{H}$ in the point group of $\mathcal{G}$ and the index of the translation group of $\mathcal{H}$ in the translation group of $\mathcal{G}$. For maximal subgroups, only one of these factors is different from 1. For *klassengleiche* subgroups, the two point groups are equal, whereas for *translationengleiche* subgroups the two translation subgroups are equal. Therefore, a maximal subgroup is easily identified either as a *klassengleiche* or a *translationengleiche* subgroup.

1.4.4. Description of the checks

In order to avoid new errors being introduced in the typesetting process after the data have been checked and corrected, we carried out the computer checks directly on the $\LaTeX\,2_\varepsilon$ sources used for the production of this volume. The tables have been typeset with specially designed $\LaTeX\,2_\varepsilon$ macros, the primary purpose of which was to guarantee a homogeneous layout throughout the book. As a side effect, it was relatively easy to write a *GAP* program which parses the $\LaTeX\,2_\varepsilon$ sources, recognizes the macros, extracts the data (the arguments of the macros), brings the data into a form suitable for further processing with routines from the *Cryst* package and finally performs the various checks. In this way, the checks could be done fully automatically, and could be repeated after every modification of the tabulated data.

In the following, we describe the checks that have been carried out. We first applied a number of tests individually to each of the tabulated maximal subgroups of low index: whether it is a subgroup, whether the index given is correct, whether the listed coordinate transformation maps the subgroup to the preferred setting of the given space-group type (and thus, whether the space-group type of the subgroup is correct) and whether the listed coordinate transformation maps the given generators of the subgroup to the standard generators of its space-group type, in the same order. Here, the preferred setting is the setting of the parent group, where applicable, and otherwise the preferred setting of the space-group type of the subgroup, if there is more than one setting in the tables.

In a second step, a complete set of maximal subgroups of low index (2, 3 or 4) is computed afresh with the routines from the *Cryst* package. These subgroups are then divided into conjugacy classes, and classified as *klassengleiche* or *translationengleiche* subgroups. This list is then compared with the tabulated list of maximal subgroups. It was verified that each maximal subgroup of a given index was listed exactly once, that the classification into conjugacy classes of subgroups was correct and that the subgroups were correctly identified as *klassengleiche* or as *translationengleiche* subgroups.

All the tests described above concern the maximal subgroups of low index. Unfortunately, similar automatic tests could not be performed on the series of isomorphic subgroups. The subgroups in these series contain variable parameters, and *Cryst* can only deal with fixed, concrete space groups without free parameters.

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1.5. The mathematical background of the subgroup tables

By Gabriele Nebe

1.5.1. Introduction

This chapter gives a brief introduction to the mathematics involved in the determination of the subgroups of space groups. To achieve this we have to detach ourselves from the geometric point of view in crystallography and introduce more abstract algebraic structures, such as coordinates, which are well known in crystallography and permit the formalization of symmetry operations, and also the abstract notion of a group, which allows us to apply general theorems to the concrete situation of (three-dimensional) space groups.

This algebraic point of view has the following advantages:

(1) Geometric problems can be treated by algebraic calculations. These calculations can be dealt with by well established procedures. In particular, the use of computers and advanced programs enables one to solve even difficult problems in a comparatively short time.

(2) The mappings form groups in the mathematical sense of the word. This means that the very powerful methods of group theory may be applied successfully.

(3) The procedures for the solution may be developed to a great extent independently of the dimension of the space.

In Section 1.5.2, a basis is laid down which gives the reader an understanding of the algebraic point of view of the crystal space (or point space) and special mappings of this space onto itself. The set of these mappings is an example of a group. For a closer connection to crystallography, the reader may consult Section 8.1.1 of *IT* A (2002) or the book by Hahn & Wondratschek (1994).

Section 1.5.3 gives an introduction to abstract groups and states the important theorems of group theory that will be applied in Section 1.5.4 to the most important groups in crystallography, the space groups. In particular, Section 1.5.4 treats maximal subgroups of space groups which have a special structure by the theorem of Hermann. In Section 1.5.5, we come back to abstract group theory stating general facts about maximal subgroups of groups. These general theorems allow us to calculate the possible indices of maximal subgroups of three-dimensional space groups in Section 1.5.6. The last section, Section 1.5.7, deals with the very subtle question of when these maximal subgroups of a space group are isomorphic to this space group.

1.5.2. The affine space

1.5.2.1. *Motivation*

The aim of this section is to give a mathematical model for the 'point space' (also known in crystallography as 'direct space' or 'crystal space') which the positions of atoms in crystals (the so-called 'points') occupy. This allows us in particular to describe the symmetry groups of crystals and to develop a formalism for calculating with these groups which has the advantage that it works in arbitrary dimensions. Such higher-dimensional spaces up to dimension 6 are used, *e.g.*, for the description of quasicrystals and incommensurate phases. For example, the more than 29 000 000 crystallographic groups up to dimension 6 can be parameterized, constructed and identified using the computer package *[CARAT]: Crystallographic AlgoRithms And Tables*, available from http://wwwb.math.rwth-aachen.de/carat/index.html.

As well as the points in point space, there are other objects, called 'vectors'. The vector that connects the point P to the point Q is usually denoted by $\overrightarrow{PQ}$. Vectors are usually visualized by arrows, where parallel arrows of the same length represent the same vector.

Whereas the sum of two points P and Q is not defined, one can add vectors. The sum $\mathbf{v}+\mathbf{w}$ of two vectors $\mathbf{v}$ and $\mathbf{w}$ is simply the sum of the two arrows. Similarly, multiplication of a vector $\mathbf{v}$ by a real number can be defined.

All the points in point space are equally good, but among the vectors one can be distinguished, the null vector $\mathbf{o}$. It is characterized by the property that $\mathbf{v}+\mathbf{o}=\mathbf{v}$ for all vectors $\mathbf{v}$.

Although the notion of a vector seems to be more complicated than that of a point, we introduce vector spaces before giving a mathematical model for the point space, the so-called affine space, which can be viewed as a certain subset of a higher-dimensional vector space, where the addition of a point and a vector makes sense.

1.5.2.2. *Vector spaces*

We shall now exploit the advantage of being independent of the dimensionality. The following definitions are independent of the dimension by replacing the specific dimensions 2 for the plane and 3 for the space by an unspecified integer number $n>0$. Although we cannot visualize four- or higher-dimensional objects, we can describe them in such a way that we are able to calculate with such objects and derive their properties.

Algebraically, an n-dimensional (real) vector $\mathbf{v}$ can be represented by a column of n real numbers. The n-dimensional real vector space $\mathbf{V}_n$ is then

$$\mathbf{V}_n=\{\boldsymbol{x}=\begin{pmatrix}x_1\\ \vdots\\ x_n\end{pmatrix}\mid x_1,\ldots,x_n\in\mathbb{R}\}.$$

(In crystallography n is normally 3.) The entries $x_1,\ldots,x_n$ are called the *coefficients* of the vector $\mathbf{x}$. On $\mathbf{V}_n$ one can naturally define an addition, where the coefficients of the sum of two vectors are the corresponding sums of the coefficients of the vectors. To multiply a vector by a real number, one just multiplies all its coefficients by this number. The null vector

$$\mathbf{o}=\begin{pmatrix}0\\ \vdots\\ 0\end{pmatrix}\in\mathbf{V}_n$$

can be distinguished, since $\mathbf{v}+\mathbf{o}=\mathbf{v}$ for all $\mathbf{v}\in\mathbf{V}_n$.

The identification of a concrete vector space $\mathbf{V}$ with the vector space $\mathbf{V}_n$ can be done by choosing a basis of $\mathbf{V}$. A *basis* of $\mathbf{V}$ is any tuple of n vectors $\mathbf{B}:=(\mathbf{a}_1,\ldots,\mathbf{a}_n)$ such that every vector of $\mathbf{V}$ can be written uniquely as a linear combination of the basis vectors: $\mathbf{V}=\{\mathbf{x}=x_1\mathbf{a}_1+\ldots+x_n\mathbf{a}_n\mid x_1,\ldots,x_n\in\mathbb{R}\}$. Whereas a vector space has many different bases, the number n of vectors of a basis is uniquely determined and is called the *dimension* of $\mathbf{V}$. The isomorphism (see Section 1.5.3.4 for a definition of isomorphism) $\varphi_{\mathbf{B}}$ between $\mathbf{V}$ and $\mathbf{V}_n$ maps the vector $\mathbf{x}=x_1\mathbf{a}_1+\ldots+x_n\mathbf{a}_n\in\mathbf{V}$

to its coefficient column

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \in \mathbf{V}_n$$

with respect to the chosen basis $\mathbf{B}$. The mapping $\varphi_{\mathbf{B}}$ respects addition of vectors and multiplication of vectors with real numbers. Moreover, $\varphi_{\mathbf{B}}$ is a bijective mapping, which means that for any coefficient column $\boldsymbol{x} \in \mathbf{V}_n$ there is a unique vector $\mathbf{x} \in \mathbf{V}$ with $\varphi_{\mathbf{B}}(\mathbf{x}) = \boldsymbol{x}$. Therefore one can perform all calculations using the coefficient columns.

An important concept in mathematics is the *automorphism group* of an object. In general, if one has an object (here the vector space $\mathbf{V}$) together with a structure (here the addition of vectors and the multiplication of vectors with real numbers), its automorphism group is the set of all one-to-one mappings of the object onto itself that preserve the structure.

A bijective mapping $\varphi : \mathbf{V} \to \mathbf{V}$ of the vector space $\mathbf{V}$ into itself satisfying $\varphi(\mathbf{v} + \mathbf{w}) = \varphi(\mathbf{v}) + \varphi(\mathbf{w})$ for all $\mathbf{v}, \mathbf{w} \in \mathbf{V}$ and $\varphi(x\mathbf{v}) = x\varphi(\mathbf{v})$ for all real numbers $x \in \mathbb{R}$ and all vectors $\mathbf{v} \in \mathbf{V}$ is called a *linear mapping* and the set of all these linear mappings is the *linear group* of $\mathbf{V}$. To know the image of $\mathbf{x} = x_1\mathbf{a}_1 + \ldots + x_n\mathbf{a}_n$ under a linear mapping φ it suffices to know the images of the basis vectors $\mathbf{a}_1, \ldots, \mathbf{a}_n$ under φ, since $\varphi(\mathbf{x}) = x_1\varphi(\mathbf{a}_1) + \ldots + x_n\varphi(\mathbf{a}_n)$. Writing the coefficient columns of the images of the basis vectors as columns of a matrix $\boldsymbol{A}$ [*i.e.* $\varphi(\mathbf{a}_i) = \sum_{j=1}^{n} \mathbf{a}_j A_{ji}$, $i = 1, \ldots, n$], then the coefficient column of $\varphi(\mathbf{x})$ with respect to the chosen basis $\mathbf{B}$ is just $\boldsymbol{A}\boldsymbol{x}$. Note that the matrix of a linear mapping depends on the basis $\mathbf{B}$ of $\mathbf{V}$. The matrix that corresponds to the composition of two linear mappings is the product of the two corresponding matrices. We have thus seen that the linear group of a vector space $\mathbf{V}$ of dimension n is isomorphic to the group of all invertible $(n \times n)$ matrices *via* the isomorphism $\phi_{\mathbf{B}}$ that associates to a linear mapping its corresponding matrix (with respect to the basis $\mathbf{B}$). This means that one can perform all calculations with linear mappings using matrix calculations.

In crystallography, the translation-vector space has an additional structure: one can measure lengths and angles between vectors. An n-dimensional real vector space with such an additional structure is called a *Euclidean vector space*, $\mathbf{E}_n$. Its automorphism group is the set of all (bijective) linear mappings of $\mathbf{E}_n$ onto itself that preserve lengths and angles and is called the *orthogonal group* $\mathcal{O}_n$ of $\mathbf{E}_n$. If one chooses the basis $\mathbf{B} = (\mathbf{e}_1, \ldots, \mathbf{e}_n)$ to be the unit vectors (which are orthogonal vectors of length 1), then the isomorphism $\phi_{\mathbf{B}}$ above maps the orthogonal group $\mathcal{O}_n$ onto the set of all $(n \times n)$ matrices $\boldsymbol{A}$ with $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \boldsymbol{I}$, the $(n \times n)$ unit matrix. $^{\mathrm{T}}$ denotes the transposition operator, which maps columns to rows and rows to columns.

1.5.2.3. *The affine space*

In this section we build up a model for the 'point space'. Let us first assume $n = 2$. Then the affine space $\mathbb{A}_2$ may be imagined as an infinite sheet of paper parallel, let us say, to the $(\mathbf{a}, \mathbf{b})$ plane and cutting the $\mathbf{c}$ axis at $x_3 = 1$ in crystallographic notation. The points of $\mathbb{A}_2$ have coordinates

$$\left(\begin{array}{c} x_1 \\ x_2 \\ \hline 1 \end{array}\right),$$

which are the coefficients of the vector from the origin to the point.

This observation is generalized by the following:

Definition 1.5.2.3.1.

$$\mathbb{A}_n := \{ \left(\begin{array}{c} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{array}\right) \mid x_i \in \mathbb{R}\} \text{ is an } n\text{-dimensional } \textit{affine space}. \quad \square$$

If

$$P = \left(\begin{array}{c} x_1 \\ \vdots \\ x_n \\ \hline 1 \end{array}\right) \text{ and } Q = \left(\begin{array}{c} y_1 \\ \vdots \\ y_n \\ \hline 1 \end{array}\right) \in \mathbb{A}_n,$$

then the vector $\overrightarrow{PQ}$ is defined as the difference

$$Q - P = \left(\begin{array}{c} y_1 - x_1 \\ \vdots \\ y_n - x_n \\ \hline 0 \end{array}\right)$$

(computed in the vector space $\mathbf{V}_{n+1}$). The set of all $\overrightarrow{PQ}$ with $P, Q \in \mathbb{A}_n$ forms an n-dimensional vector space which is called the *underlying vector space* $\tau(\mathbb{A}_n)$. Omitting the last coefficient, we can identify

$$\tau(\mathbb{A}_n) = \{ \left(\begin{array}{c} x_1 \\ \vdots \\ x_n \\ \hline 0 \end{array}\right) \mid x_1, \ldots, x_n \in \mathbb{R}\}$$

with $\mathbf{V}_n$. As the coordinates already indicate, the sets $\mathbb{A}_n$ as well as $\tau(\mathbb{A}_n)$ can be viewed as subsets of $\mathbf{V}_{n+1}$. Computed in $\mathbf{V}_{n+1}$, the sum of two elements in $\tau(\mathbb{A}_n)$ is again in $\tau(\mathbb{A}_n)$, since the last coefficient of the sum is $0 + 0 = 0$ and the sum of a point $P \in \mathbb{A}_n$ and a vector $\mathbf{v} \in \mathbf{V}_n$ is again a point in $\mathbb{A}_n$ (since the last coordinate is $1 + 0 = 1$), but the sum of two points does not make sense.

1.5.2.4. *The affine group*

The affine group of geometry is the set of all mappings of the point space which fulfil the conditions

(1) parallel straight lines are mapped onto parallel straight lines;
(2) collinear points are mapped onto collinear points and the ratio of distances between them remains constant.

In the mathematical model, the affine group is the automorphism group of the affine space and can be viewed as the set of all linear mappings of $\mathbf{V}_{n+1}$ that preserve $\mathbb{A}_n$.

Definition 1.5.2.4.1. The *affine group* $\mathcal{A}_n$ is the subset of the set of all linear mappings $\varphi : \mathbf{V}_{n+1} \to \mathbf{V}_{n+1}$ with $\varphi(\mathbb{A}_n) = \mathbb{A}_n$. The elements of $\mathcal{A}_n$ are called *affine mappings*. □

Since φ is linear, it holds that

$$\varphi(\overrightarrow{PQ}) = \varphi(Q - P) = \varphi(Q) - \varphi(P) = \overrightarrow{\varphi(P)\varphi(Q)}\,.$$

Hence an affine mapping also maps $\tau(\mathbb{A}_n)$ into itself.

Since the first n basis vectors of the chosen basis lie in $\tau(\mathbb{A}_n)$ and the last one in $\mathbb{A}_n$, it is clear that with respect to this basis the affine mappings correspond to matrices of the form

$$\mathbb{W} = \left(\begin{array}{c|c} \boldsymbol{W} & \boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right).$$

The linear mapping induced by φ on $\tau(\mathbb{A}_n)$ which is represented by the matrix $\boldsymbol{W}$ will be referred to as the *linear part* $\overline{\varphi}$ of φ. The image $\varphi(P)$ of a point P with coordinates

$$\mathbb{x} = \left(\frac{\boldsymbol{p}}{1}\right) \in \mathbb{A}_n$$

can easily be found as

$$\mathbb{W}\mathbb{x} = \left(\frac{\boldsymbol{W}\boldsymbol{p} + \boldsymbol{w}}{1}\right).$$

If one has a way to measure lengths and angles (*i.e.* a Euclidean metric) on the underlying vector space $\tau(\mathbb{A}_n)$, one can compute the *distance* between P and $Q \in \mathbb{A}_n$ as the length of the vector $\overrightarrow{PQ}$ and the angle determined by P, Q and $R \in \mathbb{A}_n$ with vertex Q is obtained from $\cos(P, Q, R) = \cos(\overrightarrow{QP}, \overrightarrow{QR})$. In this case, $\mathbb{A}_n$ is the *Euclidean affine space*, $\mathbb{E}_n$.

An affine mapping of the Euclidean affine space is called an *isometry* if its linear part is an orthogonal mapping of the Euclidean space $\tau(\mathbb{A}_n)$. The set of all isometries in $\mathcal{A}_n$ is called the *Euclidean group* and denoted by $\mathcal{E}_n$. Hence $\mathcal{E}_n$ is the set of all distance-preserving mappings of $\mathbb{E}_n$ onto itself. The isometries are the affine mappings with matrices of the form

$$\mathbb{W} = \left(\begin{array}{c|c} \boldsymbol{W} & \boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right),$$

where the linear part $\boldsymbol{W}$ belongs to the orthogonal group of $\tau(\mathbb{A}_n)$.

Special isometries are the *translations*, the isometries where the linear part is $\boldsymbol{I}$, with matrix

$$\mathbb{T}_{\boldsymbol{w}} = \left(\begin{array}{c|c} \boldsymbol{I} & \boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right).$$

The group of all translations in $\mathcal{E}_n$ is the *translation subgroup* of $\mathcal{E}_n$ and is denoted by $\mathcal{T}_n$. Note that composition of two translations means addition of the translation vectors and $\mathcal{T}_n$ is isomorphic to the translation vector space $\tau(\mathbb{E}_n)$.

1.5.3. Groups

1.5.3.1. *Groups*

The affine group is only one example of the more general concept of a group. The following axiomatic definition sometimes makes it easier to examine general properties of groups.

Definition 1.5.3.1.1. A *group* $(\mathcal{G}, \cdot)$ is a set $\mathcal{G}$ with a mapping $\cdot : \mathcal{G} \times \mathcal{G} \to \mathcal{G}; (g, h) \mapsto g \cdot h$, called the *composition law* or *multiplication* of $\mathcal{G}$, satisfying the following three axioms:

(i) $(g \cdot h) \cdot k = g \cdot (h \cdot k)$ for all $g, h, k \in \mathcal{G}$ (associative law).

(ii) There is an element $e \in \mathcal{G}$ called the *unit element* of $\mathcal{G}$ with $e \cdot g = g \cdot e = g$ for all $g \in \mathcal{G}$.

(iii) For all $g \in \mathcal{G}$, there is an element $g^{-1} \in \mathcal{G}$, called the *inverse* of g, with $g \cdot g^{-1} = g^{-1} \cdot g = e$. □

Normally the symbol $\cdot$ is omitted, hence the product $g \cdot h$ is just written as $g\,h$ and the set $\mathcal{G}$ is called a group.

One should note that in particular property (i), the associative law, of a group is something very natural if one thinks of group elements as mappings. Clearly the composition of mappings is associative. In general, one can think of groups as groups of mappings as explained in Section 1.5.3.2.

A subset of elements of a group $\mathcal{G}$ which themselves form a group is called a subgroup:

Definition 1.5.3.1.2. A non-empty subset $\emptyset \neq \mathcal{U} \subseteq \mathcal{G}$ is called a *subgroup* of $\mathcal{G}$ (abbreviated as $\mathcal{U} \leq \mathcal{G}$) if $g \cdot h^{-1} \in \mathcal{U}$ for all $g, h \in \mathcal{U}$. □

The affine group is an example of a group where $\cdot$ is given by the composition of mappings. The unit element $e \in \mathcal{A}_n$ is the identity mapping given by the matrix

$$\mathbb{I} = \left(\begin{array}{c|c} \boldsymbol{I} & \boldsymbol{o} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right),$$

which also represents the translation by the vector $\mathbf{o}$. The composition of two affine mappings is again an affine mapping and the inverse of an affine mapping $\mathbb{W}$ has matrix

$$\mathbb{W}^{-1} = \left(\begin{array}{c|c} \boldsymbol{W}^{-1} & -\boldsymbol{W}^{-1}\boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right).$$

Since the inverse of an isometry and the composition of two isometries are again isometries, the set of isometries $\mathcal{E}_n$ is a subgroup of the affine group $\mathcal{A}_n$. The translation subgroup $\mathcal{T}_n$ is a subgroup of $\mathcal{E}_n$.

Any vector space $\mathbf{V}_n$ is a group with the usual vector addition as composition law. Therefore $\tau(\mathbb{A}_n)$ is also a group.

Remarks

(i) For every group $\mathcal{G}$, the set $\{e\}$ consisting only of the unit element of $\mathcal{G}$ is a subgroup of $\mathcal{G}$ called the *trivial subgroup* $\mathcal{I} = \{e\}$.

(ii) If $\mathcal{U}$ is a subgroup of $\mathcal{V}$ and $\mathcal{V}$ is a subgroup of the group $\mathcal{G}$, then $\mathcal{U}$ is a subgroup of $\mathcal{G}$.

(iii) If $\mathcal{U}$ and $\mathcal{V}$ are subgroups of the group $\mathcal{G}$, then the intersection $\mathcal{U} \cap \mathcal{V}$ is also a subgroup of $\mathcal{G}$.

(iv) If $S \subseteq \mathcal{G}$ is a subset of the group $\mathcal{G}$, then the smallest subgroup of $\mathcal{G}$ containing S is denoted by

$$\langle S \rangle := \bigcap \{\mathcal{U} \leq \mathcal{G} \mid S \subseteq \mathcal{U}\}$$

and is called the *subgroup generated by* S. The elements of S are called the *generators* of this group. It is convenient not to list all the elements of a group $\mathcal{G}$ but just to give generators of $\mathcal{G}$ (this also applies to finite groups).

Example 1.5.3.1.3.

A well known group is the addition group of integers $\mathbb{Z} = \{0, 1, -1, 2, -2, \ldots\}$ where $\cdot$ is normally denoted by $+$ and the unit element $e \in \mathbb{Z}$ is 0. The group $\mathbb{Z}$ is generated by $\{1\}$. Other generating sets are for example $\{-1\}$ or $\{2, 3\}$. Taking two integers $a, b \in \mathbb{Z}$ which are divisible by some fixed integer $p \in \mathbb{Z}$, then the sum $a + b$ and the addition inverses $-a$ and $-b$ are again divisible by p. Hence the set $p\mathbb{Z}$ of all integers divisible by p is a subgroup of $\mathbb{Z}$. It is generated by $\{p\}$.

Definition 1.5.3.1.4. The *order* $|\mathcal{G}|$ of a group $\mathcal{G}$ is the number of elements in the set $\mathcal{G}$. □

Most of the groups $\mathcal{G}$ in crystallography, for example $\mathbb{Z}$, $\mathbf{V}_n$, $\mathcal{A}_n$, have infinite order.

Groups that are generated by one element are called *cyclic*. The cyclic group of order n is called $\mathcal{C}yc_n$. (We prefer to use three letters to denote the mathematical names of frequently occurring groups, since the more common symbol $\mathcal{C}_n$ could possibly cause confusion with the Schoenflies symbol C_n.)

The group $\mathbf{V}_n$ is not generated by a finite set.

These two groups $\mathbb{Z}$ and $\mathbf{V}_n$ have the property that for all elements g and h in the group it holds that $g \cdot h = h \cdot g$. Hence these two groups are Abelian in the sense of the following:

Definition 1.5.3.1.5. The group $(\mathcal{G}, \cdot)$ is called *Abelian* if $g \cdot h = h \cdot g$ for all $g, h \in \mathcal{G}$. □

1.5.3.2. *Actions of groups on sets*

The affine group $\mathcal{A}_n$ is defined *via* its action on the affine space $\mathbb{A}_n$. In general, the greatest significance of groups is that they act on sets.

Definition 1.5.3.2.1. Let $\mathcal{G}$ be a group. A non-empty set M is called a (*left*) $\mathcal{G}$-*set* if there is a mapping $\cdot : \mathcal{G} \times M \to M$ satisfying the following conditions:

(i) $(gh) \cdot m = g \cdot (h \cdot m)$ for all $g, h \in \mathcal{G}$ and $m \in M$.
(ii) $e \cdot m = m$ for all $m \in M$.

If M is a $\mathcal{G}$-set, one also says that $\mathcal{G}$ acts on M. □

Example 1.5.3.2.2.

(*a*) The affine space $\mathbb{A}_n$ is a $\mathcal{G}$-set for the affine group $\mathcal{G} = \mathcal{A}_n$.
(*b*) $\tau(\mathbb{A}_n)$ is an $\mathcal{A}_n$-set, where $\mathcal{A}_n$ acts *via* the linear parts.
(*c*) $\tau(\mathbb{A}_n)$ is also a group and acts on $\mathbb{A}_n$ by translations $\mathbf{v} \cdot P := P + \mathbf{v}$ for $\mathbf{v} \in \tau(\mathbb{A}_n)$, $P \in \mathbb{A}_n$.
(*d*) If $\mathcal{U} \le \mathcal{G}$ is a subgroup of the group $\mathcal{G}$, then $\mathcal{G}$ is a $\mathcal{U}$-set where $\cdot : \mathcal{U} \times \mathcal{G} \to \mathcal{G}$ is the usual composition law. In particular, each group $\mathcal{G}$ is a $\mathcal{G}$-set and hence every group $\mathcal{G}$ can be viewed as a group of mappings from $\mathcal{G}$ onto $\mathcal{G}$.

Definition 1.5.3.2.3. Let $\mathcal{G}$ be a group and M a $\mathcal{G}$-set. If $m \in M$, then the set $\mathcal{G} \cdot m := \{g \cdot m | g \in \mathcal{G}\}$ is called the *orbit* of m under $\mathcal{G}$.
The $\mathcal{G}$-set M is called *transitive* if $M = \mathcal{G} \cdot m$ for any $m \in M$ consists of a single orbit under $\mathcal{G}$.
If $m \in M$ then the *stabilizer of m in* $\mathcal{G}$ is $\mathrm{Stab}_{\mathcal{G}}(m) := \{g \in \mathcal{G} \mid g \cdot m = m\}$.
The *kernel* $\mathcal{K}$ *of the action* of $\mathcal{G}$ on M is the intersection of the stabilizers of all elements in M,

$$\mathcal{K} := \{g \in \mathcal{G} \mid g \cdot m = m \text{ for all } m \in M\}.$$

M is called a *faithful* $\mathcal{G}$-set and the action of $\mathcal{G}$ on M is also called *faithful* if the kernel of the action is trivial, $\mathcal{K} = \{e\}$. □

Remarks

(i) If $m_1, m_2 \in M$, then their orbits are either equal or disjoint. For if there is an element $g_1 \cdot m_1 = g_2 \cdot m_2$, then by the axioms of $\mathcal{G}$-sets $m_1 = em_1 = (g_1^{-1}g_1) \cdot m_1 = g_1^{-1} \cdot (g_1 \cdot m_1) = g_1^{-1} \cdot (g_2 \cdot m_2) = (g_1^{-1}g_2) \cdot m_2$, hence every element $g \cdot m_1$ in the orbit of m_1 is of the form $g \cdot (g_1^{-1}g_2 \cdot m_2) = (gg_1^{-1}g_2) \cdot m_2$ and therefore lies in the orbit of m_2. Hence the set of orbits gives a partition of M into disjoint sets. If M is a finite set, then its order is the sum of the lengths of the different orbits.
(ii) $\mathrm{Stab}_{\mathcal{G}}(m)$ is a subgroup of $\mathcal{G}$, since for $g_1, g_2 \in \mathrm{Stab}_{\mathcal{G}}(m)$, the product $(g_1g_2^{-1}) \cdot m = g_1 \cdot (g_2^{-1} \cdot m) = g_1 \cdot m = m$.
(iii) If $m_1 = g \cdot m_2$, then $\mathrm{Stab}_{\mathcal{G}}(m_1) = g\ \mathrm{Stab}_{\mathcal{G}}(m_2)g^{-1} = \{ghg^{-1} \mid h \in \mathrm{Stab}_{\mathcal{G}}(m_2)\}$.

Example 1.5.3.2.4. (Example 1.5.3.2.2 *cont.*)

(*a*) $\mathbb{A}_n$ is a transitive $\mathcal{A}_n$-set. This is a mathematical expression of the fact that in point space no point is distinguished.
(*b*) The $\mathcal{A}_n$-set $\tau(\mathbb{A}_n)$ decomposes into two orbits $\{\mathbf{o}\}$ and $\{\mathbf{v} \in \tau(\mathbb{A}_n) \mid \mathbf{v} \neq \mathbf{o}\}$. The kernel of the action of $\mathcal{A}_n$ on $\tau(\mathbb{A}_n)$ is the translation subgroup $\mathcal{T}_n$.
(*c*) $\tau(\mathbb{A}_n)$ acts transitively on $\mathbb{A}_n$. The kernel of the action only consists of the zero vector $\mathbf{o}$.

We now introduce some terminology for groups which is nicely formulated using $\mathcal{G}$-sets.

Definition 1.5.3.2.5. The orbit of $g \in \mathcal{G}$ under the action of the subgroup $\mathcal{U} \le \mathcal{G}$ is the *right coset* $\mathcal{U}g = \{ug \mid u \in \mathcal{U}\}$ (*cf. IT* A, Section 8.1.5). Analogously one defines a *left coset* as

$$g\mathcal{U} = \{gu \mid u \in \mathcal{U}\}$$

and denotes the set of left cosets by $\mathcal{G}/\mathcal{U}$.
If the number of left cosets (which is always equal to the number of right cosets) of $\mathcal{U}$ in $\mathcal{G}$ is finite, then this number is called the *index* $[\mathcal{G} : \mathcal{U}]$ of $\mathcal{U}$ in $\mathcal{G}$. If this number is infinite, one says that the index of $\mathcal{U}$ in $\mathcal{G}$ is infinite. □

Example 1.5.3.2.6.
$\mathbb{A}_n$ is a coset of $\mathbf{V}_n$ in $\mathbf{V}_{n+1}$, namely

$$\mathbb{A}_n = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \hline 1 \end{pmatrix} + \mathbf{V}_n.$$

If one thinks of $\mathbb{A}_2$ as an infinite sheet of paper and puts uncountably many such sheets of paper (one for each real number) one onto the other, one gets the whole 3-space $\mathbf{V}_3$.

Remark
The set of left cosets $\mathcal{G}/\mathcal{U}$ is a left $\mathcal{G}$-set with the operation $g \cdot (m\mathcal{U}) := (gm)\mathcal{U}$ for all $g, m \in \mathcal{G}$. The kernel of the action is the intersection of all subgroups of $\mathcal{G}$ that are conjugate to $\mathcal{U}$ and is called the *core* of $\mathcal{U}$: $\mathrm{core}(\mathcal{U}) := \bigcap_{g \in \mathcal{G}} g\mathcal{U}g^{-1}$.

We now assume that $|\mathcal{G}|$ is finite. Let $\mathcal{U} \le \mathcal{G}$ be a subgroup of $\mathcal{G}$. Then the set $\mathcal{G}$ is partitioned into left cosets of $\mathcal{U}$, $\mathcal{G} = g_1\mathcal{U} \cup \ldots \cup g_i\mathcal{U}$, where $i = [\mathcal{G} : \mathcal{U}]$ is the index of $\mathcal{U}$ in $\mathcal{G}$. Since the orders of the left cosets of $\mathcal{U}$ are all equal to the order of $\mathcal{U}$, one gets

Theorem 1.5.3.2.7. (Theorem of Lagrange.) Let $\mathcal{U}$ be a subgroup of the finite group $\mathcal{G}$. Then

$$|\mathcal{G}| = |\mathcal{U}|[\mathcal{G} : \mathcal{U}].$$

In particular, the order of any subgroup of $\mathcal{G}$ and also the index of any subgroup of $\mathcal{G}$ are divisors of the group order $|\mathcal{G}|$. □

The $\mathcal{G}$-set $\mathcal{G}/\mathcal{U}$ is only a special case of a $\mathcal{G}$-set. It is a transitive $\mathcal{G}$-set. If $M = \mathcal{G} \cdot m$ is a transitive $\mathcal{G}$-set, then the mapping $M \to \mathcal{G}/\mathrm{Stab}_{\mathcal{G}}(m), g \cdot m \mapsto g\mathrm{Stab}_{\mathcal{G}}(m)$ is a bijection (in fact an isomorphism of $\mathcal{G}$-sets in the sense of Definition 1.5.3.4.1 below). Therefore the number of elements of M, which is the length of the orbit of m under $\mathcal{G}$, equals the index of the stabilizer of m in $\mathcal{G}$, whence one gets the following generalization of the theorem of Lagrange:

Theorem 1.5.3.2.8. Let $\mathcal{G}$ be a finite group and M be a $\mathcal{G}$-set. Then

$$|\mathcal{G}| = |\mathcal{G} \cdot m||\mathrm{Stab}_{\mathcal{G}}(m)|$$

for all $m \in M$. □

Up to now, we have only considered the action of $\mathcal{G}$ upon $\mathcal{G}$ *via* multiplication. There is another natural action of $\mathcal{G}$ on itself *via conjugation*: $\mathcal{G} \times \mathcal{G} \to \mathcal{G}$ defined by $g \cdot m := gmg^{-1}$ for all group elements g and elements m in the $\mathcal{G}$-set $\mathcal{G}$. The stabilizer of m is called the *centralizer* of m in $\mathcal{G}$,

$$\mathrm{Stab}_{\mathcal{G}}(m) = \mathcal{C}_{\mathcal{G}}(m) = \{g \in \mathcal{G} \mid gmg^{-1} = m\}.$$

If $M \subset \mathcal{G}$ is a set of group elements, then the *centralizer of M* is the intersection of the centralizers of the elements in M:

$$\mathcal{C}_{\mathcal{G}}(M) = \{g \in \mathcal{G} \mid gmg^{-1} = m \text{ for all } m \in M\}.$$

Definition 1.5.3.2.9. $\mathcal{G}$ also acts on the set $\mathbf{U}$ of all subgroups of $\mathcal{G}$ by conjugation, $g \cdot \mathcal{U} := g\mathcal{U}g^{-1}$. The stabilizer of an element $\mathcal{U} \in \mathbf{U}$ is called the *normalizer of* $\mathcal{U}$ and denoted by $\mathcal{N}_{\mathcal{G}}(\mathcal{U})$. $\mathcal{U}$ is called a *normal subgroup of* $\mathcal{G}$ (denoted as $\mathcal{U} \trianglelefteq \mathcal{G}$) if $\mathcal{N}_{\mathcal{G}}(\mathcal{U}) = \mathcal{G}$. □

Remarks

(i) Let $\mathcal{U} \le \mathcal{G}$. Then the index of the normalizer in $\mathcal{G}$ of $\mathcal{U}$ is the number of subgroups of $\mathcal{G}$ that are conjugate to $\mathcal{U}$. Since $\mathcal{U}$ always normalizes itself [hence $\mathcal{U}$ is a subgroup of $\mathcal{N}_{\mathcal{G}}(\mathcal{U})$], the index of the normalizer divides the index of $\mathcal{U}$.

(ii) If $\mathcal{G}$ is Abelian, then the conjugation action of $\mathcal{G}$ is trivial, hence each subgroup of $\mathcal{G}$ is a normal subgroup.

(iii) The group $\mathcal{G}$ itself and also the trivial subgroup $\{e\} \le \mathcal{G}$ are always normal subgroups of $\mathcal{G}$.

Normal subgroups play an important role in the investigation of groups. If $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup, then the left coset $g\mathcal{N}$ equals the right coset $\mathcal{N}g$ for all $g \in \mathcal{G}$, because $g\mathcal{N} = g(g^{-1}\mathcal{N}g) = \mathcal{N}g$.

The most important property of normal subgroups is that the set of left cosets of $\mathcal{N}$ in $\mathcal{G}$ forms a group, called the *factor group* $\mathcal{G}/\mathcal{N}$, as follows: The set of all products of elements of two left cosets of $\mathcal{N}$ again forms a left coset of $\mathcal{N}$. Let $g, h \in \mathcal{G}$. Then

$$g\mathcal{N}h\mathcal{N} = g(h\mathcal{N}h^{-1})h\mathcal{N} = gh\mathcal{N}\mathcal{N} = gh\mathcal{N}.$$

This defines a natural product on the set of left cosets of $\mathcal{N}$ in $\mathcal{G}$ which turns this set into a group. The unit element is $e\mathcal{N}$.

Hence the philosophy of normal subgroups is that they cut the group into pieces, where the two pieces $\mathcal{G}/\mathcal{N}$ and $\mathcal{N}$ are again groups.

Example 1.5.3.2.10.

The group $\mathbb{Z}$ is Abelian. For any number $p \in \mathbb{Z}$, the set $p\mathbb{Z}$ is a subgroup of $\mathbb{Z}$. Hence $p\mathbb{Z}$ is a normal subgroup of $\mathbb{Z}$. The factor group $\mathbb{Z}/p\mathbb{Z}$ inherits the multiplication from the multiplication in $\mathbb{Z}$, since $ap\mathbb{Z} \subset p\mathbb{Z}$ for all $a \in \mathbb{Z}$. If p is a prime number, then all elements $\neq 0 + p\mathbb{Z}$ in $\mathbb{Z}/p\mathbb{Z}$ have a multiplicative inverse, and therefore $\mathbb{Z}/p\mathbb{Z}$ is a field, the *field with p elements*.

Proposition 1.5.3.2.11.
Let $\mathcal{N} \trianglelefteq \mathcal{G}$ be a normal subgroup of the group $\mathcal{G}$ and $\mathcal{U} \le \mathcal{G}$. Then the set

$$\mathcal{N}\mathcal{U} = \mathcal{U}\mathcal{N} := \{un \mid u \in \mathcal{U}, n \in \mathcal{N}\}$$

is a subgroup of $\mathcal{G}$. □

Proof. Let $u_1n_1, u_2n_2 \in \mathcal{U}\mathcal{N}$. Then $u_1n_1(u_2n_2)^{-1} = u_1n_1n_2^{-1}u_2^{-1} = un \in \mathcal{U}\mathcal{N}$, where $u := u_1u_2^{-1} \in \mathcal{U}$, since $\mathcal{U}$ is a subgroup of $\mathcal{G}$, and $n := u_2n_1n_2u_2^{-1} \in \mathcal{N}$, since $\mathcal{N}$ is a normal subgroup of $\mathcal{G}$. QED

1.5.3.3. *The Sylow theorems*

A nice application of the notion of $\mathcal{G}$-sets are the three theorems of Sylow. By Theorem 1.5.3.2.7, the order of any subgroup $\mathcal{U}$ of a group $\mathcal{G}$ divides the order of $\mathcal{G}$. But conversely, given a divisor d of $|\mathcal{G}|$, one cannot predict the existence of a subgroup $\mathcal{U}$ of $\mathcal{G}$ with $|\mathcal{U}| = d$. If $d = p^\beta$ is a prime power that divides $|\mathcal{G}|$, then the following theorem says that such a subgroup exists.

Theorem 1.5.3.3.1. (Sylow)
Let $\mathcal{G}$ be a finite group and p be a prime such that p^β divides the order of $\mathcal{G}$. Then $\mathcal{G}$ possesses m subgroups of order p^β, where $m > 0$ satisfies $m \equiv 1 \pmod p$. □

Theorem 1.5.3.3.2. (Sylow)
If $|\mathcal{G}| = p^\alpha s$ for some prime p not dividing s, then all subgroups of order p^α of $\mathcal{G}$ are conjugate in $\mathcal{G}$. Such a subgroup $\mathcal{U} \le \mathcal{G}$ of order $|\mathcal{U}| = p^\alpha$ is called a *Sylow p-subgroup*. □

Combining these two theorems with Theorem 1.5.3.2.8, one gets Sylow's third theorem:

Theorem 1.5.3.3.3. (Sylow)
The number of Sylow p-subgroups of $\mathcal{G}$ is $\equiv 1 \pmod p$ and divides the order of $\mathcal{G}$. □

Proofs of the three theorems above can be found in Ledermann (1976), pp.158–164.

1.5.3.4. *Isomorphisms*

If one wants to compare objects such as groups or $\mathcal{G}$-sets, to be able to say when they should be considered as equal, the concept of isomorphisms should be used:

Definition 1.5.3.4.1. Let $\mathcal{G}$ and $\mathcal{H}$ be groups and M and N be $\mathcal{G}$-sets.

(*a*) A *homomorphism* $\varphi : \mathcal{G} \to \mathcal{H}$ is a mapping of the set $\mathcal{G}$ into the set $\mathcal{H}$ respecting the composition law *i.e.* $\varphi(gh) = \varphi(g)\varphi(h)$ for all $g, h \in \mathcal{G}$.
If φ is bijective, it is called an *isomorphism* and one says $\mathcal{G}$ is *isomorphic* to $\mathcal{H}$ ($\mathcal{G} \cong \mathcal{H}$).
If $e \in \mathcal{H}$ is the unit element of $\mathcal{H}$, then the set of all pre-images of e is called the *kernel* of φ: $\ker(\varphi) := \{g \in \mathcal{G} \mid \varphi(g) = e\}$.
An isomorphism $\varphi : \mathcal{G} \to \mathcal{G}$ is called an *automorphism* of $\mathcal{G}$.

(*b*) M and N are called *isomorphic* $\mathcal{G}$-sets if there is a bijection $\varphi : M \to N$ with $g \cdot \varphi(m) = \varphi(g \cdot m)$ for all $g \in \mathcal{G}, m \in M$. □

Example 1.5.3.4.2.

In Example 1.5.3.1.3, the group homomorphism $\mathbb{Z} \to p\mathbb{Z}$ defined by $1 \mapsto p$ is a group isomorphism (from the group $\mathbb{Z}$ onto its subgroup $p\mathbb{Z}$).

Example 1.5.3.4.3.

For any group element $g \in \mathcal{G}$, conjugation by g defines an automorphism of $\mathcal{G}$. In particular, if $\mathcal{U}$ is a subgroup of $\mathcal{G}$, then $\mathcal{U}$ and its conjugate subgroup $g\mathcal{U}g^{-1}$ are isomorphic.

Philosophy: If $\mathcal{G}$ and $\mathcal{H}$ are isomorphic groups, then all group-theoretical properties of $\mathcal{G}$ and $\mathcal{H}$ are the same. The calculations in $\mathcal{G}$ can be translated by the isomorphism to calculations in $\mathcal{H}$. Sometimes it is easier to calculate in one group than in the other and translate the result back *via* the inverse of the isomorphism. For example, the isomorphism between $\tau(\mathbb{A}_n)$ and $\mathbf{V}_n$ in Section 1.5.2 is an isomorphism of groups. It even respects scalar multiplication with real numbers, so in fact it is an isomorphism of vector spaces. While the composition of translations is more concrete and easier to imagine, the calculation of the resulting vector is much easier in $\mathbf{V}_n$. The concept of isomorphism says that you can translate to the more convenient group for your calculations and translate back afterwards without losing anything.

Note that a homomorphism is injective, *i.e.* is an isomorphism onto its image, if and only if its kernel is trivial ($= \{e\}$).

Example 1.5.3.4.4.

The mapping

$$\mu : \tau(\mathbb{A}_n) \to \mathcal{A}_n, \boldsymbol{w} \mapsto \left(\begin{array}{c|c} \boldsymbol{I} & \boldsymbol{w} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array}\right)$$

is a homomorphism of the group $\tau(\mathbb{A}_n)$ into $\mathcal{A}_n$. The kernel of this homomorphism is $\{\boldsymbol{o}\}$ and the image of the mapping is the translation subgroup $\mathcal{T}_n$ of $\mathcal{A}_n$. Hence the groups $\tau(\mathbb{A}_n)$ and $\mathcal{T}_n$ are isomorphic.

The affine group acts (as group of group automorphisms) on the normal subgroup $\mathcal{T}_n \trianglelefteq \mathcal{A}_n$ *via* conjugation: $g \cdot t := gtg^{-1}$. We have seen already in Example 1.5.3.2.4 (*b*) that it also acts (as a group of linear mappings) on $\tau(\mathbb{A}_n)$. The mapping μ is an isomorphism of $\mathcal{A}_n$-sets.

1.5.3.5. *Isomorphism theorems*

[*cf.* Ledermann (1976), pp. 68–73.]

Remark

If φ is a homomorphism $\mathcal{G} \to \mathcal{H}$ and $\mathcal{N} \trianglelefteq \mathcal{H}$ is a normal subgroup of $\mathcal{H}$, then the pre-image $\varphi^{-1}(\mathcal{N}) := \{g \in \mathcal{G} \mid \varphi(g) \in \mathcal{N}\}$ is a normal subgroup of $\mathcal{G}$. In particular, it holds that $\ker(\varphi) \trianglelefteq \mathcal{G}$.

Hence the factor group $\mathcal{G}/\ker(\varphi)$ is a well defined group. The following theorem says that this group is isomorphic to the image $\varphi(\mathcal{G}) \leq \mathcal{H}$ of φ:

Theorem 1.5.3.5.1. (First isomorphism theorem.)
Let $\varphi : \mathcal{G} \to \mathcal{H}$ be a homomorphism of groups. Then

$$\overline{\varphi} : \mathcal{G}/\ker(\varphi) \to \varphi(\mathcal{G}) \leq \mathcal{H}.$$

$g\ker(\varphi) \mapsto \varphi(g)$ is an isomorphism between the factor group $\mathcal{G}/\ker(\varphi)$ and the image group of φ, which is a subgroup of $\mathcal{H}$. □

Theorem 1.5.3.5.2. (Third isomorphism theorem.)
Let $\mathcal{N} \trianglelefteq \mathcal{G}$ be a normal subgroup of the group $\mathcal{G}$ and $\mathcal{U} \leq \mathcal{G}$ be an arbitrary subgroup of $\mathcal{G}$. Then $\mathcal{U} \cap \mathcal{N} \trianglelefteq \mathcal{U}$ is a normal subgroup of $\mathcal{U}$ and

$$\mathcal{U}/(\mathcal{U} \cap \mathcal{N}) \cong \mathcal{N}\mathcal{U}/\mathcal{N}.$$

(For the definition of the group $\mathcal{N}\mathcal{U}$ see Proposition 1.5.3.2.11.) □

Definition 1.5.3.5.3. A subgroup $\mathcal{U} \leq \mathcal{H}$ is a *characteristic subgroup* $\mathcal{U}$ char $\mathcal{H}$ if $\varphi(\mathcal{U}) = \mathcal{U}$ for all automorphisms φ of $\mathcal{H}$. □

Remarks

(*a*) If $\mathcal{H}$ is a finite Abelian group and $\mathcal{P}$ is a Sylow p-subgroup of $\mathcal{H}$, then $\mathcal{P}$ char $\mathcal{H}$, because $\mathcal{P}$ is the only subgroup of $\mathcal{H}$ of order $|\mathcal{P}|$.

(*b*) If $\mathcal{H}$ is any group and $\mathcal{U}$ char $\mathcal{H}$, then $\mathcal{U} \trianglelefteq \mathcal{H}$ is also a normal subgroup of $\mathcal{H}$: for $h \in \mathcal{H}$ define the mapping $\kappa_h : \mathcal{H} \to \mathcal{H}, x \mapsto hxh^{-1}$. Then κ_h is an automorphism of $\mathcal{H}$ and $\kappa_h(\mathcal{U}) = h\mathcal{U}h^{-1} = \mathcal{U}$ since $\mathcal{U}$ is characteristic in $\mathcal{H}$.

(*c*) If $\mathcal{U}$ char $\mathcal{N} \trianglelefteq \mathcal{H}$, then $\mathcal{U} \trianglelefteq \mathcal{H}$, since the conjugation with any element of $\mathcal{H}$ induces an automorphism of $\mathcal{N}$.

1.5.3.6. *An example*

Let us consider the tetrahedral group, Schoenflies symbol T_d, which is defined as the symmetry group of a tetrahedron. It permutes the four apices P_1, P_2, P_3, P_4 of the tetrahedron and hence every element of T_d defines a bijection of $V := \{P_1, P_2, P_3, P_4\}$ onto itself. The only element that fixes all the apices is e. Therefore the set V is a faithful T_d-set. Let us calculate the order of $|T_d|$. Since there are elements in T_d that map the first apex P_1 onto each one of the other apices, V is a transitive T_d-set. Let $\mathcal{S} := \mathrm{Stab}_{T_d}(P_1)$ be the stabilizer of P_1. By Theorem 1.5.3.2.8, $|T_d| = |V||\mathcal{S}| = 4|\mathcal{S}|$. The group $\mathcal{S}$ is generated by the threefold rotation r around the 'diagonal' of the tetrahedron through P_1 and the reflection s at the symmetry plane of the tetrahedron which contains the edge (P_1, P_2). In particular, $\mathcal{S}$ acts transitively on the set $\{P_2, P_3, P_4\}$. The stabilizer of P_2 in $\mathcal{S}$ is the cyclic group $\langle s \rangle \cong \mathcal{C}yc_2$ generated by s. (The Schoenflies notation for $\langle s \rangle$ is C_s and the Hermann–Mauguin symbol is m.) Therefore $|\mathcal{S}| = 3|\langle s \rangle| = 6$ and $|T_d| = 24$. In fact, we have seen that T_d is isomorphic to the group of all bijections of V onto itself, which is the symmetric group $\mathcal{S}ym_4$ of degree 4 and the group $\mathcal{S} \cong \mathcal{S}ym_3$ is the symmetric group on $\{P_2, P_3, P_4\}$. The Schoenflies notation for $\mathcal{S}$ is C_{3v} and its Hermann–Mauguin symbol is $3m$.

In general, let $n \in \mathbb{N}$ be a natural number. Then the group of all bijective mappings of the set $\{1, \ldots, n\}$ onto itself is called the *symmetric group of degree n* and denoted by

$$\mathcal{S}ym_n := \{f : \{1, \ldots, n\} \to \{1, \ldots, n\} \mid f \text{ is bijective}\}.$$

The *alternating group* is the normal subgroup $\mathcal{A}lt_n$ consisting of all even permutations of $\{1, \ldots, n\}$.

Let us construct a normal subgroup of T_d. The tetrahedral group contains three twofold rotations r_1, r_2, r_3 around the three axes of the tetrahedron through the midpoints of opposite edges. Since T_d permutes these three axes and hence conjugates the three rotations into each other, the group

$$\mathcal{U} := \langle r_1, r_2, r_3 \rangle$$

generated by these three rotations is a normal subgroup of T_d. Since these three rotations commute with each other, the group $\mathcal{U}$ is Abelian. Now $r_1 r_2 = r_3$ and hence $\mathcal{U} = \{e, r_1, r_2, r_3\} \cong D_2$ (in Schoenflies notation) $\cong 222$ (Hermann–Mauguin symbol) is of order 4. There are three normal subgroups of order 2 in $\mathcal{U}$, namely $\langle r_i \rangle$ for $i = 1, 2, 3$. The factor group $\mathcal{U}/\langle r_1 \rangle$ is again of order 2. Since all groups of order 2 are cyclic, $\langle r_1 \rangle \cong \mathcal{U}/\langle r_1 \rangle \cong \mathcal{C}yc_2$. The set $\mathcal{U}$ is the set of all products of elements from the two normal subgroups $\langle r_1 \rangle$ and $\langle r_2 \rangle$, hence $\mathcal{U}$ is isomorphic to the *direct product* $\mathcal{C}yc_2 \times \mathcal{C}yc_2$ in the sense of the following definition.

Definition 1.5.3.6.1. [*cf.* Ledermann (1976), Section 13.] Let $\mathcal{G}$ and $\mathcal{H}$ be two groups. Then the *direct product* $\mathcal{G} \times \mathcal{H}$ is the group $\mathcal{G} \times \mathcal{H} = \{(g, h) \mid g \in \mathcal{G}, h \in \mathcal{H}\}$ with multiplication $(g, h)(g', h') := (gg', hh')$. □

Let us return to the example above. The centralizer of one of the three rotations, say of r_1, is of index 3 in T_d and hence a Sylow 2-subgroup of T_d with order 8. Following Schoenflies, we will denote this group by D_{2d} (another Schoenflies symbol for this group is S_{4v} and its Hermann–Mauguin symbol is $\bar{4}2m$).

The group $\mathcal{U}$ above is contained in D_{2d}. It is its own centralizer in T_d: $\mathcal{U} = \mathcal{C}_{T_d}(\mathcal{U})$. Therefore the factor group $T_d/\mathcal{U}$ acts faithfully (and transitively) on the set $\{r_1, r_2, r_3\}$. The stabilizer of r_1 is the subgroup D_{2d} constructed above. Using this, one easily sees that $T_d/\mathcal{U} \cong \mathcal{S}ym_3$.

Another normal subgroup in T_d is the set of all rotations in T_d. This group contains the normal subgroup $\mathcal{U}$ above of index 3 and is of index 2 in T_d (and hence has order 12). It is isomorphic to $\mathcal{A}lt_4$, the alternating group of degree 4, and has Schoenflies symbol T and Hermann–Mauguin symbol 23.

1.5.4. Space groups

1.5.4.1. *Definition of space groups*

In *IT* A (2002), Section 8.1.6, space groups are introduced as symmetry groups of crystal patterns.

Definition 1.5.4.1.1.

(*a*) Let $\mathbf{V}_n$ be the *n*-dimensional real vector space. A subset $\mathbf{L} \subseteq \mathbf{V}_n$ is called an (*n*-dimensional) *lattice* if there is a basis $(\mathbf{b}_1, \ldots, \mathbf{b}_n)$ of $\mathbf{V}_n$ such that

$$\mathbf{L} = \mathbb{Z}\mathbf{b}_1 + \ldots + \mathbb{Z}\mathbf{b}_n = \{\sum_{i=1}^{n} a_i \mathbf{b}_i \mid a_i \in \mathbb{Z}\}.$$

(*b*) A *crystal structure* is a mapping $f : \mathbb{E}_n \to \mathbb{R}$ of the Euclidean affine *n*-space into the real numbers such that $\mathrm{Stab}_{\tau(\mathbb{A}_n)}(f) := \{t \in \tau(\mathbb{A}_n) \mid f(P+t) = f(P) \text{ for all } P \in \mathbb{A}_n\}$ is an *n*-dimensional lattice in $\tau(\mathbb{A}_n)$.

(*c*) The Euclidean group $\mathcal{E}_n$ acts on the set of mappings $\mathbb{E}_n \to \mathbb{R}$ *via* $(g \cdot f)(P) := f(g^{-1}P)$ for all $P \in \mathbb{E}_n$ and for all $g \in \mathcal{E}_n$ and $f : \mathbb{E}_n \to \mathbb{R}$. A *space group* $\mathcal{R}$ is the stabilizer of a crystal structure $f : \mathbb{E}_n \to \mathbb{R}$; $\mathcal{R} = \mathrm{Stab}_{\mathcal{E}_n}(f)$.

(*d*) Let $\mathcal{R} \le \mathcal{E}_n$ be a space group. The *translation subgroup* $\mathcal{T}(\mathcal{R})$ of $\mathcal{R}$ is defined as $\mathcal{T}(\mathcal{R}) := \mathcal{R} \cap \mathcal{T}_n$. □

The definition introduced space groups in the way they occur in crystallography: The group of symmetries of an ideal crystal stabilizes the crystal structure. This definition is not very helpful in analysing the structure of space groups. If $\mathcal{R}$ is a space group, then the translation subgroup $\mathcal{T} := \mathcal{T}(\mathcal{R})$ is a normal subgroup of $\mathcal{R}$. It is even a characteristic subgroup of $\mathcal{R}$, hence fixed under every automorphism of $\mathcal{R}$. By Definition 1.5.4.1.1, its image under the inverse μ' of the mapping μ in Example 1.5.3.4.4 defined by

$$\mu' : \mathcal{T} \to \tau(\mathbb{E}_n); \left(\begin{array}{c|c} \boldsymbol{I} & \boldsymbol{v} \\ \hline \boldsymbol{o}^{\mathrm{T}} & 1 \end{array} \right) \mapsto \boldsymbol{v}$$

in $\tau(\mathbb{A}_n)$ is a full lattice $\mathbf{L}(\mathcal{R})$. Since μ' is an isomorphism from $\mathcal{T}$ onto $\mathbf{L}(\mathcal{R})$, the translation subgroup of $\mathcal{R}$ is isomorphic to the lattice $\mathbf{L}(\mathcal{R})$. In particular, one has $\mu'(t_1 t_2) = \mu'(t_1) + \mu'(t_2)$ and the subgroup $\mathcal{T}^p$, formed by the *p*th powers of elements in $\mathcal{T}$, is mapped onto $p\mathbf{L}(\mathcal{R})$. Lattices are well understood. Although they are infinite, they have a simple structure, so they can be examined algorithmically. Since they lie in a vector space, one can apply linear algebra to them.

Now we want to look at how this lattice $\mathcal{T}(\mathcal{R})$ fits into the space group $\mathcal{R}$. The affine group $\mathcal{A}_n$ acts on $\mathcal{T}_n$ by conjugation as well as on $\tau(\mathbb{A}_n)$ *via* its linear part. Similarly the space group $\mathcal{R}$ acts on $\mathcal{T}(\mathcal{R})$ by conjugation: For $g \in \mathcal{R}$ and $t \in \mathcal{T}$, one gets $\mu'(gtg^{-1}) = \overline{g}\mu'(t)$, where $\overline{g}$ is the linear part of g. Therefore the kernel of this action is on the one hand the centralizer of $\mathcal{T}(\mathcal{R})$ in $\mathcal{R}$, on the other hand, since $\mathbf{L}(\mathcal{R})$ contains a basis of $\tau(\mathbb{E}_n)$, it is equal to the kernel of the mapping $\bar{\ }$, which is $\mathcal{R} \cap \mathcal{T}_n = \mathcal{T}(\mathcal{R})$, hence

$$\mathcal{C}_{\mathcal{R}}(\mathcal{T}(\mathcal{R})) = \mathcal{T}(\mathcal{R}).$$

Hence only the linear part $\overline{\mathcal{R}} \cong \mathcal{R}/\mathcal{T}(\mathcal{R})$ of $\mathcal{R}$ acts faithfully on $\mathcal{T}(\mathcal{R})$ by conjugation and linearly on $\mathbf{L}(\mathcal{R})$. This factor group $\mathcal{R}/\mathcal{T}(\mathcal{R})$ is a finite group. Let us summarize this:

Theorem 1.5.4.1.2. Let $\mathcal{R}$ be a space group. The translation subgroup $\mathcal{T}(\mathcal{R}) = \mathcal{R} \cap \mathcal{T}_n$ is an Abelian normal subgroup of $\mathcal{R}$ which is its own centralizer, $\mathcal{C}_{\mathcal{R}}(\mathcal{T}(\mathcal{R})) = \mathcal{T}(\mathcal{R})$. The finite group $\mathcal{R}/\mathcal{T}(\mathcal{R})$ acts faithfully on $\mathcal{T}(\mathcal{R})$ by conjugation. This action is similar to the action of the linear part $\overline{\mathcal{R}}$ on the lattice $\mu'(\mathcal{T}(\mathcal{R})) = \mathbf{L}(\mathcal{R})$. □

1.5.4.2. *Maximal subgroups of space groups*

Definition 1.5.4.2.1. A subgroup $\mathcal{M} \le \mathcal{G}$ of a group $\mathcal{G}$ is called *maximal* if $\mathcal{M} \ne \mathcal{G}$ and for all subgroups $\mathcal{U} \le \mathcal{G}$ with $\mathcal{M} \subseteq \mathcal{U}$ it holds that either $\mathcal{U} = \mathcal{M}$ or $\mathcal{U} = \mathcal{G}$. □

The translation subgroup $\mathcal{T} := \mathcal{T}(\mathcal{R})$ of the space group $\mathcal{R}$ plays a very important role if one wants to analyse the space group $\mathcal{R}$. Let $\mathcal{U} \ne \mathcal{R}$ be a subgroup of $\mathcal{R}$. Then $\mathcal{U}$ has either fewer translations ($\mathcal{T}(\mathcal{U}) < \mathcal{T}$) or the order of the linear part of $\mathcal{U}$, the index of $\mathcal{T}(\mathcal{U})$ in $\mathcal{U}$, gets smaller ($|\overline{\mathcal{U}}| < |\overline{\mathcal{R}}|$), or both happen.

Definition 1.5.4.2.2. Let $\mathcal{U}$ be a subgroup of the space group $\mathcal{R}$ and $\mathcal{T} := \mathcal{T}(\mathcal{R})$.

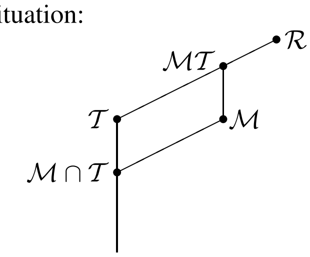
(*t*) $\mathcal{U}$ is called a *translationengleiche* or a *t-subgroup* if $\mathcal{U} \cap \mathcal{T} = \mathcal{T}$.

(*k*) $\mathcal{U}$ is called a *klassengleiche* or a *k-subgroups* if $\mathcal{U}/\mathcal{U} \cap \mathcal{T} \cong \mathcal{R}/\mathcal{T}$. □

Remark

The third isomorphism theorem, Theorem 1.5.3.5.2, implies that if $\mathcal{U}$ is a *k*-subgroup, then $\mathcal{U}\mathcal{T}/\mathcal{T} \cong \mathcal{U}/\mathcal{U} \cap \mathcal{T} \cong \mathcal{R}/\mathcal{T}$. Hence $\mathcal{U}$ is a *k*-subgroup if and only if $\mathcal{U}\mathcal{T} = \mathcal{R}$.

Let $\mathcal{M}$ be a maximal subgroup of $\mathcal{R}$. Then we have the following preliminary situation:

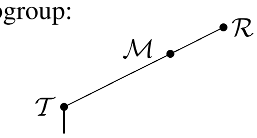


Since $\mathcal{T} \trianglelefteq \mathcal{R}$ and $\mathcal{M} \le \mathcal{R}$, one has by Proposition 1.5.3.2.11 that $\mathcal{M}\mathcal{T} \le \mathcal{R}$. Hence the maximality of $\mathcal{M}$ implies that $\mathcal{M}\mathcal{T} = \mathcal{M}$ or $\mathcal{M}\mathcal{T} = \mathcal{R}$. If $\mathcal{M}\mathcal{T} = \mathcal{M}$ then $\mathcal{T} \subseteq \mathcal{M}$, hence $\mathcal{M}$ is a *t*-subgroup. If $\mathcal{M}\mathcal{T} = \mathcal{R}$, then by the third isomorphism theorem, Theorem 1.5.3.5.2, $\mathcal{R}/\mathcal{T} = \mathcal{M}\mathcal{T}/\mathcal{T} \cong \mathcal{M}/(\mathcal{M} \cap \mathcal{T}) = \mathcal{M}/\mathcal{T}(\mathcal{M})$, hence $\mathcal{M}$ is a *k*-subgroup. This is given by the following theorem:

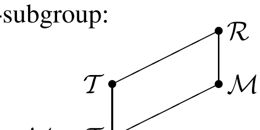
Theorem 1.5.4.2.3. (Hermann) Let $\mathcal{M} \le \mathcal{R}$ be a maximal subgroup of the space group $\mathcal{R}$. Then $\mathcal{M}$ is either a *k*-subgroup or a *t*-subgroup. □

The above picture looks as follows in the two cases:

t-subgroup:



k-subgroup:



Let $\mathcal{M}$ be a *t*-subgroup of $\mathcal{R}$. Then $\mathcal{T}(\mathcal{R}) \le \mathcal{M}$ and $\mathcal{M}/\mathcal{T}(\mathcal{R})$ is a subgroup $\mathcal{S}$ of $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$. On the other hand, any subgroup $\mathcal{S}$ of $\mathcal{P}$ defines a unique *t*-subgroup $\mathcal{M}$ of $\mathcal{R}$ with $\mathcal{T}(\mathcal{R}) \le \mathcal{M}$ and $\mathcal{M}/\mathcal{T}(\mathcal{R}) = \mathcal{S}$, namely $\mathcal{M} = \{s \in \mathcal{R} \mid s\mathcal{T}(\mathcal{R}) \in \mathcal{S}\}$. Hence the *t*-subgroups of $\mathcal{R}$ are in bijection to the subgroups of $\mathcal{P}$, which is a finite group according to the remarks below Definition 1.5.4.1.1. For future reference, we note this in the following corollary:

Corollary 1.5.4.2.4. The *t*-subgroups of the space group $\mathcal{R}$ are in bijection with the subgroups of the finite group $\mathcal{R}/\mathcal{T}(\mathcal{R})$. □

In the case $n = 3$, which is the most important case in crystallography, the finite groups $\mathcal{R}/\mathcal{T}(\mathcal{R})$ are isomorphic to subgroups of either $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ (Hermann–Mauguin symbol $m\overline{3}m$) or $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ (= $6/mmm$). Here $\times$ denotes the direct product (*cf.* Definition 1.5.3.6.1), $\mathcal{C}yc_2$ the cyclic group of order 2, and $\mathcal{S}ym_3$ and $\mathcal{S}ym_4$ the symmetric groups of degree 3 or 4, respectively (*cf.* Section 1.5.3.6). Hence the maximal subgroups $\mathcal{M}$ of $\mathcal{R}$ that are *t*-subgroups can be read off from the subgroups of the two groups above.

An algorithm for calculating the maximal t-subgroups of $\mathcal{R}$ which applies to all three-dimensional space groups is explained in Section 1.5.5.

The more difficult task is the determination of the maximal k-subgroups.

Lemma 1.5.4.2.5. Let $\mathcal{M}$ be a maximal k-subgroup of the space group $\mathcal{R}$. Then $\mathcal{T}(\mathcal{M}) = \mathcal{T} \cap \mathcal{M} \trianglelefteq \mathcal{R}$ is a normal subgroup of $\mathcal{R}$. Hence $\mu'(\mathcal{T}(\mathcal{M})) \leq \mathbf{L}(\mathcal{R})$ is an $\overline{\mathcal{R}}$-invariant lattice. □

Proof. $\mathcal{R} = \mathcal{T}\mathcal{M}$, so every element g in $\mathcal{R}$ can be written as $g = tm$ where $t \in \mathcal{T}$ and $m \in \mathcal{M}$. Therefore one obtains for $t_1 \in \mathcal{T} \cap \mathcal{M}$

$$g^{-1} t_1 g = m^{-1} t^{-1} t_1 t m = m^{-1} t_1 m,$$

since $\mathcal{T}$ is Abelian. Since $m \in \mathcal{R}$ and $\mathcal{T}$ is normal in $\mathcal{R}$, one has $m^{-1} t_1 m \in \mathcal{T}$. But $m^{-1} t_1 m$ is a product of elements in $\mathcal{M}$ and therefore lies in the subgroup $\mathcal{M}$, hence $m^{-1} t_1 m \in \mathcal{T} \cap \mathcal{M}$. QED

The candidates for translation subgroups $\mathcal{T}(\mathcal{M})$ of maximal k-subgroups $\mathcal{M}$ of $\mathcal{R}$ can be found by linear-algebra algorithms using the philosophy explained at the beginning of this section: $\mathcal{R}$ acts on $\mathcal{T}$ by conjugation and this action is isomorphic to the action of the linear part $\overline{\mathcal{R}} \cong \mathcal{R}/\mathcal{T}$ of $\mathcal{R}$ on the lattice $\mathbf{L}(\mathcal{R})$ *via* the isomorphism $\mu' : \mathcal{T} \to \mathbf{L}(\mathcal{R})$. Normal subgroups of $\mathcal{R}$ contained in $\mathcal{T}$ are mapped onto $\overline{\mathcal{R}}$-invariant sublattices of $\mathbf{L}(\mathcal{R})$. An example for such a normal subgroup is the group $\mathcal{T}^p$ formed by the pth powers of elements of $\mathcal{T}$ for any natural number $p \in \mathbb{N}$. One has $\mu'(\mathcal{T}^p) = p\mathbf{L}(\mathcal{R})$.

If $\mathcal{M}$ is a maximal k-subgroup of $\mathcal{R}$, then $\mathcal{T}(\mathcal{M})$ is a normal subgroup of $\mathcal{R}$ that is maximal in $\mathcal{T}$, which means that $\mu'(\mathcal{T}(\mathcal{M})) = \mathbf{L}(\mathcal{M})$ is a maximal $\overline{\mathcal{R}}$-invariant sublattice of $\mathbf{L}(\mathcal{R})$. Hence it contains $p\mathbf{L}(\mathcal{R})$ for some prime number p. One may view $\mathcal{T}/\mathcal{T}^p \cong \mathbf{L}(\mathcal{R})/p\mathbf{L}(\mathcal{R})$ as a finite $(\mathbb{Z}/p\mathbb{Z})\overline{\mathcal{R}}$-module and find all candidates for such normal subgroups as full pre-images of maximal $(\mathbb{Z}/p\mathbb{Z})\overline{\mathcal{R}}$-submodules of $\mathbf{L}(\mathcal{R})/p\mathbf{L}(\mathcal{R})$. This gives an algorithm for calculating these normal subgroups, which is implemented in the package *[CARAT]*.

The group $\mathcal{G} := \mathcal{T}/\mathcal{T}^p$ is an Abelian group, with the additional property that for all $g \in \mathcal{G}$ one has $g^p = e$. Such a group is called an *elementary Abelian p-group*.

From the reasoning above we find the following lemma.

Lemma 1.5.4.2.6. Let $\mathcal{M}$ be a maximal k-subgroup of the space group $\mathcal{R}$. Then $\mathcal{T}/\mathcal{T}(\mathcal{M})$ is an elementary Abelian p-group for some prime p. The order of $\mathcal{T}/\mathcal{T}(\mathcal{M})$ is p^r with $r \leq n$. □

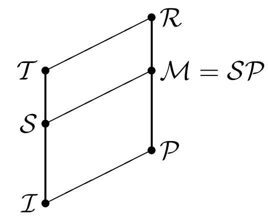
Corollary 1.5.4.2.7. Maximal subgroups of space groups are again space groups and of finite index in the supergroup. □

Hence the first step is the determination of subgroups of $\mathcal{R}$ that are maximal in $\mathcal{T}$ and normal in $\mathcal{R}$, and is solved by linear-algebra algorithms. These subgroups are the candidates for the translation subgroups $\mathcal{T}(\mathcal{M})$ for maximal k-subgroups $\mathcal{M}$. But even if one knows the isomorphism type of $\mathcal{M}/\mathcal{T}(\mathcal{M})$, the group $\mathcal{T}(\mathcal{M})$ does not in general determine $\mathcal{M} \leq \mathcal{R}$. Given such a normal subgroup $\mathcal{S} \trianglelefteq \mathcal{R}$ that is contained in $\mathcal{T}$, one now has to find all maximal k-subgroups $\mathcal{M} \leq \mathcal{R}$ with $\mathcal{S} = \mathcal{T} \cap \mathcal{M}$ and $\mathcal{T}\mathcal{M} = \mathcal{R}$. It might happen that there is no such group $\mathcal{M}$. This case does not occur if $\mathcal{R}$ is a symmorphic space group in the sense of the following definition:

Definition 1.5.4.2.8. A space group $\mathcal{R}$ is called *symmorphic* if there is a subgroup $\mathcal{P} \leq \mathcal{R}$ such that $\mathcal{P} \cap \mathcal{T}(\mathcal{R}) = \mathcal{I}$ and $\mathcal{P}\mathcal{T}(\mathcal{R}) = \mathcal{R}$. The subgroup $\mathcal{P}$ is called a *complement* of the translation subgroup $\mathcal{T}(\mathcal{R})$. □

Note that the group $\mathcal{P}$ in the definition is isomorphic to $\mathcal{R}/\mathcal{T}(\mathcal{R})$ and hence a finite group.

If $\mathcal{R}$ is symmorphic and $\mathcal{P} \leq \mathcal{R}$ is a complement of $\mathcal{T}$, then one may take $\mathcal{M} := \mathcal{S}\mathcal{P}$.



This shows the following:

Lemma 1.5.4.2.9. Let $\mathcal{R}$ be a symmorphic space group with translation subgroup $\mathcal{T}$ and $\mathcal{T}_1 \leq \mathcal{T}$ an $\mathcal{R}$-invariant subgroup of $\mathcal{T}$ (*i.e.* $\mathcal{T}_1 \trianglelefteq \mathcal{R}$). Then there is at least one k-subgroup $\mathcal{U} \leq \mathcal{R}$ with translation subgroup $\mathcal{T}_1$. □

In any case, the maximal k-subgroups, $\mathcal{M}$, of $\mathcal{R}$ satisfy
$\mathcal{M}\mathcal{T} = \mathcal{R}$ and
$\mathcal{M} \cap \mathcal{T} = \mathcal{S}$ is a maximal $\mathcal{R}$-invariant subgroup of $\mathcal{T}$.

To find these maximal subgroups, $\mathcal{M}$, one first chooses such a subgroup $\mathcal{S}$. It then suffices to compute in the finite group $\mathcal{R}/\mathcal{S} =: \overline{\mathcal{R}}$. If there is a complement $\overline{\mathcal{M}}$ of $\overline{\mathcal{T}} = \mathcal{T}/\mathcal{S}$ in $\overline{\mathcal{R}}$, then every element $x \in \overline{\mathcal{R}}$ may be written uniquely as $x = mt$ with $m \in \overline{\mathcal{M}}$, $t \in \overline{\mathcal{T}}$. In particular, any other complement $\overline{\mathcal{M}'}$ of $\overline{\mathcal{T}}$ in $\overline{\mathcal{R}}$ is of the form $\overline{\mathcal{M}'} = \{mt_m \mid m \in \overline{\mathcal{M}}, t_m \in \overline{\mathcal{T}}\}$. One computes $m_1 t_{m_1} m_2 t_{m_2} = m_1 m_2 (m_2^{-1} t_{m_1} m_2) t_{m_2}$. Since $\overline{\mathcal{M}'}$ is a subgroup of $\overline{\mathcal{R}}$, it holds that $t_{m_1 m_2} = (m_2^{-1} t_{m_1} m_2) t_{m_2}$. Moreover, every mapping $\overline{\mathcal{M}} \to \overline{\mathcal{T}}; m \mapsto t_m$ with this property defines some maximal subgroup $\mathcal{M}'$ as above. Since $\overline{\mathcal{M}}$ and $\overline{\mathcal{T}}$ are finite, it is a finite problem to find all such mappings.

If there is no such complement $\overline{\mathcal{M}}$, this means that there is no (maximal) k-subgroup $\mathcal{M}$ of $\mathcal{R}$ with $\mathcal{M} \cap \mathcal{T} = \mathcal{S}$.

1.5.5. Maximal subgroups

1.5.5.1. *Maximal subgroups and primitive $\mathcal{G}$-sets*

To determine the maximal t-subgroups of a space group $\mathcal{R}$, essentially one has to calculate the maximal subgroups of the finite group $\mathcal{R}/\mathcal{T}(\mathcal{R})$. There are fast algorithms to calculate these maximal subgroups if this finite group is soluble (see Definition 1.5.5.2.1), which is the case for three-dimensional space groups. To explain this method and obtain theoretical consequences for the index of maximal subgroups in soluble space groups, we consider abstract groups again in this section.

For an arbitrary group $\mathcal{G}$, one has a fast method of checking whether a given subgroup $\mathcal{U} \leq \mathcal{G}$ of finite index $[\mathcal{G} : \mathcal{U}]$ is maximal by inspection of the $\mathcal{G}$-set $\mathcal{G}/\mathcal{U}$ of left cosets of $\mathcal{U}$ in $\mathcal{G}$. Assume that $\mathcal{U} \leq \mathcal{M} \leq \mathcal{G}$ and let $\mathcal{M}/\mathcal{U} := \{m_1\mathcal{U}, \ldots, m_k\mathcal{U}\}$ with $m_i \in \mathcal{M}$, $m_1 = e$ and $\mathcal{G}/\mathcal{M} := \{g_1\mathcal{M}, \ldots, g_l\mathcal{M}\}$ with $g_i \in \mathcal{G}$, $g_1 = e$. Then the set $\mathcal{G}/\mathcal{U}$ may be written as

$$\begin{array}{rlll} \mathcal{G}/\mathcal{U} = & \{g_1 m_1 \mathcal{U}, & \ldots, & g_1 m_k \mathcal{U}, \\ & g_2 m_1 \mathcal{U}, & \ldots, & g_2 m_k \mathcal{U}, \\ & \vdots, & \ldots, & \vdots, \\ & g_l m_1 \mathcal{U}, & \ldots, & g_l m_k \mathcal{U}\} \end{array}.$$

Then $\mathcal{G}$ permutes the lines of the rectangle above: For all $g \in \mathcal{G}$ and all $j \in \{1, \ldots, l\}$, the left coset $gg_j\mathcal{M}$ is equal to some $g_a\mathcal{M}$

for an $a \in \{1, \ldots, l\}$. Hence the jth line is mapped onto the set

$$\{gg_j m_1 \mathcal{U}, \ldots, gg_j m_k \mathcal{U}\} = \{g_a m_1 \mathcal{U}, \ldots, g_a m_k \mathcal{U}\}.$$

Definition 1.5.5.1.1. Let $\mathcal{G}$ be a group and X a $\mathcal{G}$-set.

(i) A *congruence* $\{S_1, \ldots, S_l\}$ on X is a partition of X into non-empty subsets $X = \dot\bigcup_{i=1}^{l} S_i$ such that for all $x_1, x_2 \in S_i$, $g \in \mathcal{G}$, $gx_1 \in S_j$ implies $gx_2 \in S_j$.

(ii) The congruences $\{X\}$ and $\{\{x\} \mid x \in X\}$ are called the *trivial congruences*.

(iii) X is called a *primitive* $\mathcal{G}$-set if $\mathcal{G}$ is transitive on X, $|X| > 1$ and X has only the trivial congruences. □

Hence the considerations above have proven the following lemma.

Lemma 1.5.5.1.2. Let $\mathcal{M} \leq \mathcal{G}$ be a subgroup of the group $\mathcal{G}$. Then $\mathcal{M}$ is a maximal subgroup if and only if the $\mathcal{G}$-set $\mathcal{G}/\mathcal{M}$ is primitive. □

The advantage of this point of view is that the groups $\mathcal{G}$ having a faithful, primitive, finite $\mathcal{G}$-set have a special structure. It will turn out that this structure is very similar to the structure of space groups.

If X is a $\mathcal{G}$-set and $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup of $\mathcal{G}$, then $\mathcal{G}$ acts on the set of $\mathcal{N}$-orbits on X, hence $\{\mathcal{N}x \mid x \in X\}$ is a congruence on X. If X is a primitive $\mathcal{G}$-set, then this congruence is trivial, hence $\mathcal{N}x = \{x\}$ or $\mathcal{N}x = X$ for all $x \in X$. This means that $\mathcal{N}$ either acts trivially or transitively on X.

One obtains the following:

Theorem 1.5.5.1.3. [Theorem of Galois (*ca* 1830).]
Let $\mathcal{H}$ be a finite group and let X be a faithful, primitive $\mathcal{H}$-set. Assume that $\{e\} \neq \mathcal{N} \trianglelefteq \mathcal{H}$ is an Abelian normal subgroup. Then

(*a*) $\mathcal{N}$ is a minimal normal subgroup of $\mathcal{H}$ (*i.e.* for all $\mathcal{N}_1 \trianglelefteq \mathcal{H}$, $\mathcal{N}_1 \subseteq \mathcal{N} \Leftrightarrow \mathcal{N}_1 = \mathcal{N}$ or $\mathcal{N}_1 = \{e\}$).

(*b*) $\mathcal{N}$ is an elementary Abelian p-group for some prime p and $|X| = |\mathcal{N}|$ is a prime power.

(*c*) $\mathcal{C}_{\mathcal{H}}(\mathcal{N}) = \mathcal{N}$ and $\mathcal{N}$ is the unique minimal normal subgroup of $\mathcal{H}$. □

Proof. Let $\{e\} \neq \mathcal{N} \trianglelefteq \mathcal{H}$ be an Abelian normal subgroup. Then $\mathcal{N}$ acts faithfully and transitively on X. To establish a bijection between the sets $\mathcal{N}$ and X, choose $x \in X$ and define $\varphi : \mathcal{N} \to X; n \mapsto n \cdot x$. Since $\mathcal{N}$ is transitive, φ is surjective. To show the injectivity of φ, let $n_1, n_2 \in \mathcal{N}$ with $\varphi(n_1) = \varphi(n_2)$. Then $n_1 \cdot x = n_2 \cdot x$, hence $n_1^{-1} n_2 x = x$. But then $n_1^{-1} n_2$ acts trivially on X, because if $y \in X$ then the transitivity of $\mathcal{N}$ implies that there is an $n \in \mathcal{N}$ with $n \cdot x = y$. Then $n_1^{-1} n_2 \cdot y = n_1^{-1} n_2 n \cdot x = n n_1^{-1} n_2 \cdot x = n \cdot x = y$, since $\mathcal{N}$ is Abelian. Since X is a faithful $\mathcal{H}$-set, this implies $n_1^{-1} n_2 = e$ and therefore $n_1 = n_2$. This proves $|\mathcal{N}| = |X|$. Since this equality holds for all nontrivial Abelian normal subgroups of $\mathcal{H}$, statement (*a*) follows. If p is some prime dividing $|\mathcal{N}|$, then the Sylow p-subgroup of $\mathcal{N}$ is normal in $\mathcal{N}$, since $\mathcal{N}$ is Abelian. Therefore it is also a characteristic subgroup of $\mathcal{N}$ and hence a normal subgroup in $\mathcal{H}$ (see the remarks below Definition 1.5.3.5.3). Since $\mathcal{N}$ is a minimal normal subgroup of $\mathcal{H}$, this implies that $\mathcal{N}$ is equal to its Sylow p-subgroup. Therefore, the order of $\mathcal{N}$ is a prime power $|\mathcal{N}| = p^r$ for some prime p and $r \in \mathbb{N}$. Similarly, the set $\mathcal{N}^p := \{n^p \mid n \in \mathcal{N}\}$ is a normal subgroup of $\mathcal{H}$ properly contained in $\mathcal{N}$. Therefore $\mathcal{N}^p = \{e\}$ and $\mathcal{N}$ is elementary Abelian. This establishes (*b*).
To see that (*c*) holds, let $g \in \mathcal{C}_{\mathcal{H}}(\mathcal{N})$. Choose $x \in X$. Then $g \cdot x = y \in X$. Since $\mathcal{N}$ acts transitively, there is an $n \in \mathcal{N}$ such that $n \cdot x = y$. Hence $n^{-1} g \cdot x = x$. As above, let $z \in X$ be any element of X. Then there is an element $n_1 \in \mathcal{N}$ with $z = n_1 \cdot x$. Hence $n^{-1} g \cdot z = n^{-1} g n_1 \cdot x = n_1 n^{-1} g \cdot x = n_1 \cdot x = z$. Since z was arbitrary and X is faithful, this implies that $g = n \in \mathcal{N}$. Therefore $\mathcal{C}_{\mathcal{H}}(\mathcal{N}) \subseteq \mathcal{N}$. Since $\mathcal{N}$ is Abelian, one has $\mathcal{N} \subseteq \mathcal{C}_{\mathcal{H}}(\mathcal{N})$, hence $\mathcal{N} = \mathcal{C}_{\mathcal{H}}(\mathcal{N})$. To see that $\mathcal{N}$ is unique, let $\mathcal{P} \neq \mathcal{N}$ be another normal subgroup of $\mathcal{H}$. Since $\mathcal{N}$ is a minimal normal subgroup, one has $\mathcal{N} \cap \mathcal{P} = \{e\}$, and therefore for $p \in \mathcal{P}$, $n \in \mathcal{N}$: $n^{-1} p^{-1} n p \in \mathcal{N} \cap \mathcal{P} = \{e\}$. Hence $\mathcal{P}$ centralizes $\mathcal{N}$, $\mathcal{P} \subseteq \mathcal{C}_{\mathcal{H}}(\mathcal{N}) = \mathcal{N}$, which is a contradiction. QED

Hence the groups $\mathcal{H}$ that satisfy the hypotheses of the theorem of Galois are certain subgroups of an affine group $\mathcal{A}_n(\mathbb{Z}/p\mathbb{Z})$ over a finite field $\mathbb{Z}/p\mathbb{Z}$. This affine group is defined in a way similar to the affine group $\mathcal{A}_n$ over the real numbers where one has to replace the real numbers by this finite field. Then $\mathcal{N}$ is the translation subgroup of $\mathcal{A}_n(\mathbb{Z}/p\mathbb{Z})$ isomorphic to the n-dimensional vector space

$$(\mathbb{Z}/p\mathbb{Z})^{\,n} = \{\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \mid x_1, \ldots, x_n \in \mathbb{Z}/p\mathbb{Z}\}$$

over $\mathbb{Z}/p\mathbb{Z}$. The set X is the corresponding affine space $\mathbb{A}_n(\mathbb{Z}/p\mathbb{Z})$. The factor group $\overline{\mathcal{H}} = \mathcal{H}/\mathcal{N}$ is isomorphic to a subgroup of the linear group of $(\mathbb{Z}/p\mathbb{Z})^n$ that does not leave invariant any non-trivial subspace of $(\mathbb{Z}/p\mathbb{Z})^n$.

1.5.5.2. *Soluble groups*

Definition 1.5.5.2.1. Let $\mathcal{G}$ be a group. The *derived series* of $\mathcal{G}$ is the series $(\mathcal{G}_0, \mathcal{G}_1, \ldots)$ defined *via* $\mathcal{G}_0 := \mathcal{G}$, $\mathcal{G}_i := \langle g^{-1} h^{-1} g h \mid g, h \in \mathcal{G}_{i-1} \rangle$. The group $\mathcal{G}_1$ is called the *derived subgroup* of $\mathcal{G}$. The group $\mathcal{G}$ is called *soluble* if $\mathcal{G}_n = \{e\}$ for some $n \in \mathbb{N}$. □

Remarks

(i) The $\mathcal{G}_i$ are characteristic subgroups of $\mathcal{G}$.

(ii) $\mathcal{G}$ is Abelian if and only if $\mathcal{G}_1 = \{e\}$.

(iii) $\mathcal{G}_1$ is characterized as the smallest normal subgroup of $\mathcal{G}$, such that $\mathcal{G}/\mathcal{G}_1$ is Abelian, in the sense that every normal subgroup of $\mathcal{G}$ with an Abelian factor group contains $\mathcal{G}_1$.

(iv) Subgroups and factor groups of soluble groups are soluble.

(v) If $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup, then $\mathcal{G}$ is soluble if and only if $\mathcal{G}/\mathcal{N}$ and $\mathcal{N}$ are both soluble.

Example 1.5.5.2.2.
The derived series of $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ is:

$$\mathcal{C}yc_2 \times \mathcal{S}ym_4 \trianglerighteq \mathcal{A}lt_4 \trianglerighteq \mathcal{C}yc_2 \times \mathcal{C}yc_2 \trianglerighteq \mathcal{I}$$

(or in Hermann–Mauguin notation $m\overline{3}m \trianglerighteq 23 \trianglerighteq 222 \trianglerighteq 1$) and that of $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ is

$$\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3 \trianglerighteq \mathcal{C}yc_3 \trianglerighteq \mathcal{I}$$

(Hermann–Mauguin notation: $6/mmm \trianglerighteq 3 \trianglerighteq 1$).
Hence these two groups are soluble. (For an explanation of the groups that occur here and later, see Section 1.5.3.6.)

Now let $\mathcal{R} \leq \mathcal{E}_3$ be a three-dimensional space group. Then $\mathcal{T}(\mathcal{R})$ is an Abelian normal subgroup, hence $\mathcal{T}(\mathcal{R})$ is soluble. The factor group $\mathcal{R}/\mathcal{T}(\mathcal{R})$ is isomorphic to a subgroup of either $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ or $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ and therefore also soluble. Using the remark above, one deduces that all three-dimensional space groups are soluble.

Lemma 1.5.5.2.3. Let $\mathcal{R}$ be a three-dimensional space group. Then $\mathcal{R}$ is soluble. □

1.5.5.3. *Maximal subgroups of soluble groups*

Now let $\mathcal{G}$ be a soluble group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup of finite index in $\mathcal{G}$. Then the set of left cosets $X := \mathcal{G}/\mathcal{M}$ is a primitive finite $\mathcal{G}$-set. Let $\mathcal{K} = \mathrm{core}(\mathcal{M})$ be the kernel of the action of $\mathcal{G}$ on X. Then the factor group $\mathcal{H} := \mathcal{G}/\mathcal{K}$ acts faithfully on X. In particular, $\mathcal{H}$ is a finite group and X is a primitive, faithful $\mathcal{H}$-set. Since $\mathcal{G}$ is soluble, the factor group $\mathcal{H}$ is also a soluble group. Let $\mathcal{H} \trianglerighteq \mathcal{H}_1 \trianglerighteq \ldots \trianglerighteq \mathcal{H}_{n-1} \trianglerighteq \{e\}$ be the derived series of $\mathcal{H}$ with $\mathcal{N} := \mathcal{H}_{n-1} \neq \{e\}$. Then $\mathcal{N}$ is an Abelian normal subgroup of $\mathcal{H}$. The theorem of Galois (Theorem 1.5.5.1.3) states that $\mathcal{N}$ is an elementary Abelian p-group for some prime p and $|X| = |\mathcal{N}| = p^r$ for some $r \in \mathbb{N}$. Since $X = \mathcal{G}/\mathcal{M}$, the order of X is the index $[\mathcal{G} : \mathcal{M}]$ of $\mathcal{M}$ in $\mathcal{G}$. Therefore one gets the following theorem:

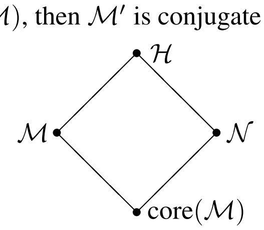
Theorem 1.5.5.3.1. If $\mathcal{M} \leq \mathcal{G}$ is a maximal subgroup of finite index in the soluble group $\mathcal{G}$, then its index $|\mathcal{G}/\mathcal{M}|$ is a prime power. □

In the proof of Theorem 1.5.5.1.3, we have established a bijection between $\mathcal{N}$ and the $\mathcal{H}$-set X, which is now $X := \mathcal{G}/\mathcal{M}$. Taking the full pre-image

$$\mathcal{N}' := \mathcal{N}\mathrm{core}(\mathcal{M})$$

of $\mathcal{N}$ in $\mathcal{G}$, then one has $\mathcal{G} = \mathcal{N}'\mathcal{M}$ and $\mathcal{M} \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$. Hence we have seen the first part of the following theorem:

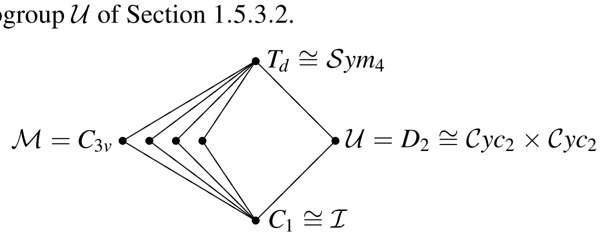
Theorem 1.5.5.3.2. Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of the soluble group $\mathcal{G}$. Then the factor group $\mathcal{H} := \mathcal{G}/\mathrm{core}(\mathcal{M})$ acts primitively and faithfully on $X := \mathcal{G}/\mathcal{M}$, and there is a normal subgroup $\mathcal{N}' \trianglelefteq \mathcal{G}$ with $\mathcal{M}\mathcal{N}' = \mathcal{G}$ and $\mathcal{M} \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$. Moreover, if $\mathcal{M}'$ is another subgroup of $\mathcal{G}$, with $\mathcal{M}'\mathcal{N}' = \mathcal{G}$ and $\mathcal{M}' \cap \mathcal{N}' = \mathrm{core}(\mathcal{M})$, then $\mathcal{M}'$ is conjugate to $\mathcal{M}$.



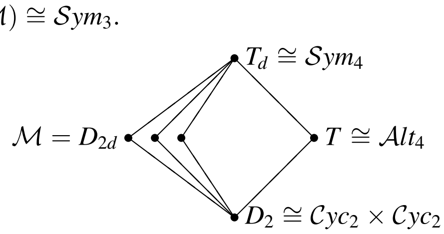
□

Example 1.5.5.3.3.

$\mathcal{G} = \mathcal{S}ym_4 \cong T_d$ is the tetrahedral group from Section 1.5.3.2 and $\mathcal{S}ym_3 \cong \mathcal{M} = C_{3v} \leq \mathcal{G}$ is the stabilizer of one of the four apices in the tetrahedron. Then $\mathrm{core}(\mathcal{M}) = \{e\}$ and $\mathcal{G}/\mathcal{M}$ is a faithful $\mathcal{G}$-set which can be identified with the set of apices of the tetrahedron. The normal subgroup $\mathcal{N} = \mathcal{N}'$ is the normal subgroup $\mathcal{U}$ of Section 1.5.3.2.



Now let $\mathcal{G} = \mathcal{S}ym_4 \cong T_d$ be as above, and take $D_{2d} \cong \mathcal{M} \leq \mathcal{G}$ a Sylow 2-subgroup of $\mathcal{G}$. Then $\mathrm{core}(\mathcal{M}) = D_2 \cong \mathcal{C}yc_2 \times \mathcal{C}yc_2$ is the normal subgroup $\mathcal{U}$ from Section 1.5.3.2 and $\mathcal{H} = \mathcal{G}/\mathrm{core}(\mathcal{M}) \cong \mathcal{S}ym_3$.



These observations result in an algorithm for computing maximal subgroups of soluble groups $\mathcal{G}$:

compute normal subgroups $\mathcal{C}$ [candidates for $\mathrm{core}(\mathcal{M})$];
compute a minimal normal subgroup $\mathcal{N}/\mathcal{C}$ of $\mathcal{G}/\mathcal{C}$;
find $\mathcal{M}/\mathcal{C}$ as a complement of $\mathcal{N}/\mathcal{C}$ in $\mathcal{G}/\mathcal{C}$.

1.5.6. Quantitative results

This section gives estimates for the number of maximal subgroups of a given index in space groups.

1.5.6.1. *General results*

The first very easy but useful remark applies to general groups $\mathcal{G}$:

Remark
Let $\mathcal{M} \leq \mathcal{G}$ be a maximal subgroup of $\mathcal{G}$ of finite index $i := [\mathcal{G} : \mathcal{M}] < \infty$. Then $\mathcal{M} \leq \mathcal{N}_{\mathcal{G}}(\mathcal{M}) \leq \mathcal{G}$. Hence the maximality of $\mathcal{M}$ implies that either $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{G}$ and $\mathcal{M}$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{N}_{\mathcal{G}}(\mathcal{M}) = \mathcal{M}$ and $\mathcal{G}$ has i maximal subgroups that are conjugate to $\mathcal{M}$.

The smallest possible index of a proper subgroup is 2. It is well known and easy to see that subgroups of index 2 are normal subgroups:

Proposition 1.5.6.1.1. Let $\mathcal{G}$ be a group and $\mathcal{M} \leq \mathcal{G}$ a subgroup of index $2 = |\mathcal{G}/\mathcal{M}|$. Then $\mathcal{M}$ is a normal subgroup of $\mathcal{G}$. □

Proof. Choose an element $g \in \mathcal{G}$, $g \notin \mathcal{M}$. Then $\mathcal{G} = \mathcal{M} \cup g\mathcal{M} = \mathcal{M} \cup \mathcal{M}g$. Hence $g\mathcal{M} = \mathcal{M}g$ and therefore $g\mathcal{M}g^{-1} = \mathcal{M}$. Since this is also true if $g \in \mathcal{M}$, the proposition follows. QED

Let $\mathcal{M}$ be a subgroup of a group $\mathcal{G}$ of index 2. Then $\mathcal{M} \trianglelefteq \mathcal{G}$ is a normal subgroup and the factor group $\mathcal{G}/\mathcal{M}$ is a group of order 2. Since groups of order 2 are Abelian, it follows that the derived subgroup $\mathcal{G}_1$ of $\mathcal{G}$ (*cf.* Definition 1.5.5.2.1) (which is the smallest normal subgroup of $\mathcal{G}$ such that the factor group is Abelian) is contained in $\mathcal{M}$. Hence all maximal subgroups of index 2 in $\mathcal{G}$ contain $\mathcal{G}_1$. If one defines $\mathcal{N} := \cap\{\mathcal{M} \leq \mathcal{G} \mid [\mathcal{G} : \mathcal{M}] = 2\}$, then $\mathcal{G}/\mathcal{N}$ is an elementary Abelian 2-group and hence a vector space over the field with two elements. The maximal subgroups of $\mathcal{G}/\mathcal{N}$ are the maximal subspaces of this vector space, hence their number is $2^a - 1$, where $a := \dim_{\mathbb{Z}/2\mathbb{Z}}(\mathcal{G}/\mathcal{N})$.

This shows the following:

Corollary 1.5.6.1.2. The number of subgroups of $\mathcal{G}$ of index 2 is of the form $2^a - 1$ for some $a \geq 0$. □

Dealing with subgroups of index 3, one has the following:

Proposition 1.5.6.1.3. Let $\mathcal{U}$ be a subgroup of the group $\mathcal{G}$ with $[\mathcal{G} : \mathcal{U}] = 3$. Then $\mathcal{U}$ is either a normal subgroup of $\mathcal{G}$ or $\mathcal{G}/\mathrm{core}(\mathcal{U}) \cong \mathcal{S}_3$ and there are three subgroups of $\mathcal{G}$ conjugate to $\mathcal{U}$. □

Proof. $\mathcal{G}/\mathrm{core}(\mathcal{U})$ is isomorphic to a subgroup of $\mathcal{S}ym_3$ that acts primitively on $\{1, 2, 3\}$. Hence either $\mathcal{G}/\mathrm{core}(\mathcal{U}) \cong \mathcal{C}yc_3$ and $\mathcal{U} = \mathrm{core}(\mathcal{U})$ is a normal subgroup of $\mathcal{G}$ or $\mathcal{G}/\mathrm{core}(\mathcal{U}) \cong \mathcal{S}ym_3$, $\mathcal{U}/\mathrm{core}(\mathcal{U}) \cong \mathcal{C}yc_2$ and there are three subgroups of $\mathcal{G}$ conjugate to $\mathcal{U}$. QED

1.5.6.2. *Three-dimensional space groups*

We now come to space groups. By Lemma 1.5.5.2.3, all three-dimensional space groups are soluble. Theorem 1.5.5.3.1 says that the index of a maximal subgroup of a soluble group is a prime power (or infinite). Since the index of a maximal subgroup of a space group is always finite (see Corollary 1.5.4.2.7), we get:

Corollary 1.5.6.2.1. Let $\mathcal{G}$ be a three-dimensional space group and $\mathcal{M} \leq \mathcal{G}$ a maximal subgroup. Then $[\mathcal{G} : \mathcal{M}]$ is a prime power. □

Let $\mathcal{R}$ be a three-dimensional space group and $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$ its point group. It is well known that the order of $\mathcal{P}$ is of the form $2^a 3^b$ with $a = 0, 1, 2, 3$ or 4 and $b = 0, 1$. By Corollary 1.5.4.2.4, the *t*-subgroups of $\mathcal{R}$ are in one-to-one correspondence with the subgroups of $\mathcal{P}$. Let us look at the *t*-subgroups of $\mathcal{R}$ of index 3. It is clear that $\mathcal{P}$ has no subgroup of index 3 if $b = 0$, since the index of a subgroup divides the order of the finite group $\mathcal{P}$ by the theorem of Lagrange. If $b = 1$, then any subgroup $\mathcal{S}$ of $\mathcal{P}$ of index 3 has order $|\mathcal{P}|/3 = 2^a$ and hence is a Sylow 2-subgroup of $\mathcal{P}$. Therefore there is such a subgroup $\mathcal{S}$ of index 3 in $\mathcal{P}$ by the first theorem of Sylow, Theorem 1.5.3.3.1. By the second theorem of Sylow, Theorem 1.5.3.3.2, all these Sylow 2-subgroups of $\mathcal{P}$ are conjugate in $\mathcal{P}$. Therefore, by Proposition 1.5.6.1.3, the number of these groups is either 1 or 3:

Corollary 1.5.6.2.2. Let $\mathcal{R}$ be a three-dimensional space group.

If the order of the point group of $\mathcal{R}$ is not divisible by 3 then $\mathcal{R}$ has no *t*-subgroups of index 3.

If 3 is a factor of the order of the point group of $\mathcal{R}$, then $\mathcal{R}$ has either one *t*-subgroup of index 3 (which is then normal in $\mathcal{R}$) or three conjugate *t*-subgroups of index 3. □

1.5.7. Qualitative results

1.5.7.1. *General theory*

In this section, we want to comment on the very subtle question of deciding whether two space groups $\mathcal{R}_1$ and $\mathcal{R}_2$ are isomorphic.

This problem can be treated in several stages:

Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be space groups. Since the translation subgroups $\mathcal{T}(\mathcal{R}_i)$ are characteristic subgroups of $\mathcal{R}_i$ (the maximal Abelian normal subgroup of finite index), each isomorphism $\varphi : \mathcal{R}_1 \to \mathcal{R}_2$ induces isomorphisms of the corresponding translation subgroups

$$\varphi' : \mathcal{T}(\mathcal{R}_1) \to \mathcal{T}(\mathcal{R}_2)$$

(by restriction) as well as of the point groups

$$\overline{\varphi} : \mathcal{P}_1 := \mathcal{R}_1/\mathcal{T}(\mathcal{R}_1) \to \mathcal{R}_2/\mathcal{T}(\mathcal{R}_2) =: \mathcal{P}_2.$$

It is convenient to view $\mathcal{T}(\mathcal{R}_i)$ as a lattice on which the point group $\mathcal{P}_i$ acts as group of linear mappings (*cf.* the start of Section 1.5.4). Then the isomorphism φ' is an isomorphism of $\mathcal{P}_1$-sets, where $\mathcal{P}_1$ acts on $\mathcal{T}(\mathcal{R}_1)$ *via* conjugation and on $\mathcal{T}(\mathcal{R}_2)$ *via*

$$g\mathcal{T}(\mathcal{R}_1) \cdot t := \varphi(g)t\varphi(g)^{-1} \text{ for all } g\mathcal{T}(\mathcal{R}_1) \in \mathcal{P}_1, t \in \mathcal{T}(\mathcal{R}_2).$$

Since $\varphi(\mathcal{T}(\mathcal{R}_1)) = \mathcal{T}(\mathcal{R}_2)$ and $\mathcal{T}(\mathcal{R}_2)$ centralizes itself, this action is well defined, *i.e.* independent of the choice of the coset representative g.

The following theorem will show that the isomorphism of sufficiently large factor groups of $\mathcal{R}_1$ and $\mathcal{R}_2$ implies a 'near' isomorphism of the space groups themselves. To give a precise formulation we need one further definition.

Definition 1.5.7.1.1. For $d \in \mathbb{N}$ define

$$O_d := \{\frac{a}{b} \mid a, b \in \mathbb{Z}, b \neq 0, \gcd(b, d) = 1\} \leq \mathbb{Q},$$

which is the set of all rational numbers for which the denominator is prime to d. For the space group $\mathcal{R} \leq \mathcal{E}_n$ let $\mathcal{R} \leq \mathcal{R}_{(d)} \leq \mathcal{E}_n$ be the group $\mathcal{R}_{(d)} := \langle \mathcal{T}(\mathcal{R})_{(d)}, \mathcal{R} \rangle$, where

$$\mathcal{T}(\mathcal{R})_{(d)} = \{at \mid a \in O_{(d)}, t \in \mathcal{T}(\mathcal{R})\} \leq \mathcal{T}_n,$$

i.e. one allows denominators that are prime to d in the translation subgroup. □

One has the following:

Theorem 1.5.7.1.2. Let $\mathcal{R}_1$ and $\mathcal{R}_2$ be two space groups with point groups of order $d_i := |\mathcal{R}_i/\mathcal{T}(\mathcal{R}_i)|$. Let $\mathbf{N}(\mathcal{R}_i)$ denote the set of normal subgroups of $\mathcal{R}_i$ having finite index in $\mathcal{R}_i$. Then the following three conditions are equivalent:

(i) There are normal subgroups $\mathcal{S}_i \trianglelefteq \mathcal{R}_i$ with $\mathcal{R}_1/\mathcal{S}_1 \cong \mathcal{R}_2/\mathcal{S}_2$ and with $\mathcal{S}_i \subseteq d_i^2\mathcal{T}(\mathcal{R}_i)$ if $d_i \neq 2$ and $\mathcal{S}_i \subseteq 16\mathcal{T}(\mathcal{R}_i)$ if $d_i = 2$ $(i = 1, 2)$.

(ii) $(\mathcal{R}_1)_{(d_1)} \cong (\mathcal{R}_2)_{(d_2)}$.

(iii) There is a bijection $\mu : \mathbf{N}(\mathcal{R}_1) \to \mathbf{N}(\mathcal{R}_2)$ such that $\mathcal{R}_1/\mathcal{N} \cong \mathcal{R}_2/\mu(\mathcal{N})$ for all $\mathcal{N} \in \mathbf{N}(\mathcal{R}_1)$. □

For a proof of this theorem, see Finken *et al.* (1980).

Remark

If $\mathcal{R}_i$ are three- or four-dimensional space groups, the isomorphism in (ii) already implies the isomorphism of $\mathcal{R}_1$ and $\mathcal{R}_2$, but there are counterexamples for dimension 5.

1.5.7.2. *Three-dimensional space groups*

Corollary 1.5.7.2.1. Let $\mathcal{R}$ be a three-dimensional space group with translation subgroup $\mathcal{T}$ and p be a prime not dividing the order of the point group $\mathcal{R}/\mathcal{T}$. Let $\mathcal{U}$ be a subgroup of $\mathcal{R}$ of index p^α for some $\alpha \in \mathbb{Z}_{>0}$. Then

(*a*) $\mathcal{U}$ is a *k*-subgroup.

(*b*) $\mathcal{U}$ is isomorphic to $\mathcal{R}$. □

Proof:

(*a*) $\mathcal{U} \leq \mathcal{U}\mathcal{T} \leq \mathcal{R}$ implies that $[\mathcal{R} : \mathcal{U}\mathcal{T}]$ divides $[\mathcal{R} : \mathcal{U}] = p^\alpha$. Since $\mathcal{T} \leq \mathcal{U}\mathcal{T} \leq \mathcal{R}$, one obtains $[\mathcal{R} : \mathcal{U}\mathcal{T}]$ as a factor of $[\mathcal{R} : \mathcal{T}]$. But p is not a factor of $[\mathcal{R} : \mathcal{T}]$, hence $[\mathcal{R} : \mathcal{U}\mathcal{T}] = 1$ and $\mathcal{R} = \mathcal{U}\mathcal{T}$. According to the remark following Definition 1.5.4.2.2, $\mathcal{U}$ is a *k*-subgroup.

(*b*) Let $d_1 := |\mathcal{R}/\mathcal{T}| = |\mathcal{U}/\mathcal{T}(\mathcal{U})|$. Let $d := d_1^2$ if $d_1 \neq 2$ and $d := 16$ otherwise, and let $\mathcal{T}' := d\mathcal{T}$. Since $\gcd([\mathcal{R} : \mathcal{U}], d) = 1$, one has $\mathcal{U}\mathcal{T}' = \mathcal{R}$ and $\mathcal{T}' \cap \mathcal{U} = d\mathcal{T}(\mathcal{U})$. By the third isomorphism theorem, Theorem 1.5.3.5.2, it follows that

$$\mathcal{R}/\mathcal{T}' = \mathcal{U}\mathcal{T}'/\mathcal{T}' \cong \mathcal{U}/\mathcal{T}' \cap \mathcal{U} = \mathcal{U}/d\mathcal{T}(\mathcal{U}).$$

By Theorem 1.5.7.1.2 (i) ⇒ (ii), one has $\mathcal{R}_{(d_1)} \cong \mathcal{U}_{(d_1)}$. By the remark above, this already implies that $\mathcal{R}$ and $\mathcal{U}$ are isomorphic. QED

Theorem 1.5.7.2.2. Let $\mathcal{R}$ be a three-dimensional space group and $\mathcal{U}$ be a maximal subgroup of $\mathcal{R}$ of index > 4. Then

(*a*) $\mathcal{U}$ is a *k*-subgroup.

(*b*) $\mathcal{U}$ is isomorphic to $\mathcal{R}$. □

Proof. Since $\mathcal{R}$ is soluble, the index $[\mathcal{R} : \mathcal{U}] = p^\alpha$ is a prime power (see Theorem 1.5.5.3.1). If p is not a factor of $|\mathcal{R}/\mathcal{T}(\mathcal{R})|$, the statement follows from Corollary 1.5.7.2.1. Hence we only have to consider the cases $p = 2$, $\alpha > 2$ and $p = 3$, $\alpha > 1$. Since 9 is not a factor of the order of any crystallographic point group in dimension 3, assertion (*a*) follows if the index of $\mathcal{U}$ is divisible by 9. If $\mathcal{U}$ is a maximal *t*-subgroup, then $\mathcal{R}/\mathcal{U}$ is a primitive $\mathcal{P}$-set for the point group $\mathcal{P}$ of $\mathcal{R}$. Since the point groups $\mathcal{P}$ of dimension 3 have no primitive $\mathcal{P}$-sets of order divisible by 8, assertion (*a*) also follows if the index of $\mathcal{U}$ is divisible by 8.

For all three-dimensional space groups $\mathcal{R}$, the module $\mathbf{L}(\mathcal{R})/2\mathbf{L}(\mathcal{R})$ [where $\mathcal{T}(\mathcal{R})$ is identified with the corresponding lattice $\mathbf{L}(\mathcal{R})$ in $\tau(\mathbb{E}_3)$ as in Section 1.5.4] is not simple as a module for the point group $\mathcal{P} = \mathcal{R}/\mathcal{T}(\mathcal{R})$. [It suffices to check this property for the two maximal point groups $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ ($= m\overline{3}m$) and $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$ ($= 6/mmm$).] This means that $2\mathbf{L}(\mathcal{R})$ is not a maximal $\mathcal{R}$-invariant sublattice of $\mathbf{L}(\mathcal{R})$. Since the translation subgroup $\mathcal{T}(\mathcal{U})$ of a maximal *k*-subgroup $\mathcal{U}$ of index equal to a power of 2 in $\mathcal{R}$ is a maximal $\mathcal{R}$-invariant subgroup of $\mathcal{T}(\mathcal{R})$ that contains $2\mathcal{T}(\mathcal{R})$, one now finds that $\mathcal{R}$ has no maximal *k*-subgroup of index 8.

Now assume that $[\mathcal{R} : \mathcal{U}] = 9$. By Corollary 1.5.7.2.1, one only needs to deal with groups $\mathcal{R}$ such that the order of the point group $\mathcal{P} := \mathcal{R}/\mathcal{T}(\mathcal{R})$ is divisible by 3. $\mathcal{P}$ is isomorphic to a subgroup of $\mathcal{C}yc_2 \times \mathcal{S}ym_4$ or $\mathcal{C}yc_2 \times \mathcal{C}yc_2 \times \mathcal{S}ym_3$. If $\mathcal{A}lt_4 \leq \mathcal{P}$ is a subgroup of $\mathcal{P}$, then $\mathbf{L}(\mathcal{R})/3\mathbf{L}(\mathcal{R})$ is simple and $\mathcal{U}$ is of index 27 in $\mathcal{R}$ [with $\mathbf{L}(\mathcal{U}) = 3\mathbf{L}(\mathcal{R})$]. It turns out that $\mathcal{U}$ is isomorphic to $\mathcal{R}$ in these cases. If $\mathcal{P}$ does not contain a subgroup isomorphic to $\mathcal{A}lt_4$, then the maximality of $\mathcal{U}$ implies that $\mathcal{T}(\mathcal{U}) \leq \mathcal{T}(\mathcal{R})$ is of index 3 in $\mathcal{T}(\mathcal{R})$. Hence $[\mathcal{R} : \mathcal{U}] = 3$ in this case. QED

Corollary 1.5.7.2.3. Let $\mathcal{M}$ be a maximal subgroup of the three-dimensional space group $\mathcal{R}$.

(*a*) If the index of $\mathcal{M}$ is a power of 2, then $[\mathcal{R} : \mathcal{M}] = 2$ or 4.

(*b*) If 3 is a factor of the order of the point group $[\mathcal{R} : \mathcal{T}(\mathcal{R})]$ and the index of $\mathcal{M}$ is a power of 3, then $[\mathcal{R} : \mathcal{M}] = 3$ or 27. For $[\mathcal{R} : \mathcal{M}] = 27$, $\mathcal{M}$ is necessarily isomorphic to $\mathcal{R}$ (by Theorem 1.5.7.2.2). □

This interesting fact explains why there are no maximal subgroups of index 8 in a three-dimensional space group. If there is a maximal subgroup $\mathcal{M}$ of a three-dimensional space group $\mathcal{R}$ of index 9, then the order of the point group of $\mathcal{R}$ is not divisible by three and the subgroup $\mathcal{M}$ is a *k*-subgroup and isomorphic to $\mathcal{R}$.

In particular, there are no maximal subgroups of index 9 for trigonal, hexagonal or cubic space groups, whereas there are such subgroups of tetragonal space groups.

2.1. Guide to the subgroup tables and graphs

BY HANS WONDRATSCHEK AND MOIS I. AROYO

2.1.1. Contents and arrangement of the subgroup tables

In this chapter, the subgroup tables, the subgroup graphs and their general organization are discussed. In the following sections, the different types of data are explained in detail. For every plane group and every space group there is a separate table of maximal subgroups and minimal supergroups. These items are listed either individually, or as members of (infinite) series, or both. In addition, there are graphs of *translationengleiche* and *klassengleiche* subgroups which contain for each space group all kinds of subgroups, not just the maximal ones.

The presentation of the plane-group and space-group data in the tables of Chapters 2.2 and 2.3 follows the style of the tables of Parts 6 (plane groups) and 7 (space groups) in Vol. A of *International Tables for Crystallography* (2002), henceforth abbreviated as *IT* A. The data comprise:

Headline
Generators selected
General position
I Maximal *translationengleiche* subgroups
II Maximal *klassengleiche* subgroups
I Minimal *translationengleiche* supergroups
II Minimal non-isomorphic *klassengleiche* supergroups.

For the majority of groups, the data can be listed completely on one page. Sometimes two pages are needed. If the data extend less than half a page over one full page and data for a neighbouring space-group table 'overflow' to a similar extent, then the two overflows are displayed on the same page. Such deviations from the standard sequence are indicated on the relevant pages by a remark *Continued on* …. The two overflows are separated by a rule and are designated by their headlines.

The sequence of the plane groups and space groups $\mathcal{G}$ in this volume follows exactly that of the tables of Part 6 (plane groups) and Part 7 (space groups) in *IT* A. The format of the subgroup tables has also been chosen to resemble that of the tables of *IT* A as far as possible. Examples of graphs of subgroups can also be found in Section 10.1.4.3 of *IT* A, but only for subgroups of point groups. The graphs for the space groups are described in Section 2.1.7.

2.1.2. Structure of the subgroup tables

Some basic data in these tables have been repeated from the tables of *IT* A in order to allow the use of the subgroup tables independently of *IT* A. These data and the main features of the tables are described in this section. More detailed descriptions are given in the following sections.

2.1.2.1. *Headline*

The headline contains the specification of the space group for which the maximal subgroups are considered. The headline lists from the outside margin inwards:

(1) The *short (international) Hermann–Mauguin symbol* for the plane group or space group. These symbols will be henceforth referred to as 'HM symbols'. HM symbols are discussed in detail in Chapter 12.2 of *IT* A with a brief summary in Section 2.2.4 of *IT* A.

(2) The plane-group or space-group number as introduced in *International Tables for X-ray Crystallography*, Vol. I (1952). These numbers run from 1 to 17 for the plane groups and from 1 to 230 for the space groups.

(3) The *full (international) Hermann–Mauguin symbol* for the plane or space group, abbreviated 'full HM symbol'. This describes the symmetry in up to three symmetry directions (*Blickrichtungen*) more completely, see Table 12.3.4.1 of *IT* A, which also allows comparison with earlier editions of *International Tables*.

(4) The *Schoenflies symbol* for the space group (there are no Schoenflies symbols for the plane groups). The Schoenflies symbols are primarily point-group symbols; they are extended by superscripts for a unique designation of the space-group types, *cf.* *IT* A, Sections 12.1.2 and 12.2.2.

2.1.2.2. *Data from IT A*

2.1.2.2.1. *Generators selected*

As in *IT* A, for each plane group and space group $\mathcal{G}$ a set of symmetry operations is listed under the heading 'Generators selected'. From these group elements, $\mathcal{G}$ can be generated conveniently. The generators in this volume are the same as those in *IT* A. They are explained in Section 2.2.10 of *IT* A and the choice of the generators is explained in Section 8.3.5 of *IT* A.

The generators are listed again in this present volume because many of the subgroups are characterized by their generators. These (often nonconventional) generators of the subgroups can thus be compared with the conventional ones without reference to *IT* A.

2.1.2.2.2. *General position*

Like the generators, the general position has also been copied from *IT* A, where an explanation can be found in Section 2.2.11. The general position in *IT* A is the first block under the heading 'Positions', characterized by its site symmetry of 1. The elements of the general position have the following meanings:

(1) they are coset representatives of the space group $\mathcal{G}$. The other elements of a coset are obtained from its representative by combination with translations of $\mathcal{G}$;

(2) they form a kind of shorthand notation for the matrix description of the coset representatives of $\mathcal{G}$;

(3) they are the coordinates of those symmetry-equivalent points that are obtained by the application of the coset representatives on a point with the coordinates x, y, z;

(4) their numbers refer to the geometric description of the symmetry operations in the block 'Symmetry operations' of the space-group tables of *IT* A.

Many of the subgroups $\mathcal{H}$ in these tables are characterized by the elements of their general position. These elements are specified by numbers which refer to the corresponding numbers in the general position of $\mathcal{G}$. Other subgroups are listed by the numbers of their generators, which again refer to the corresponding numbers in the general position of $\mathcal{G}$. Therefore, the listing of the general position of $\mathcal{G}$ as well as the listing of the generators of $\mathcal{G}$ is essential for the structure of these tables. For examples, see Sections 2.1.3 and 2.1.4.

2.1.2.3. *Specification of the setting*

All 17 plane-group types[1] and 230 space-group types are listed and described in *IT* A. However, whereas each plane-group type is represented exactly once, 44 space-group types, *i.e.* nearly 20%, are represented twice. This means that the conventional setting of these 44 space-group types is not uniquely determined and must be specified. The same settings underlie the data of this volume, which follows *IT* A as much as possible.

There are three reasons for listing a space-group type twice:

(1) Each of the 13 monoclinic space-group types is listed twice, with 'unique axis *b*' and 'unique axis *c*', where *b* or *c* is the direction distinguished by symmetry (*monoclinic axis*). The tables of this Part 2 always refer to the conventional cell choice, *i.e.* 'cell choice 1', whereas in *IT* A for each setting three cell choices are shown. In the graphs, the monoclinic space groups are designated by their short HM symbols.
Note on standard monoclinic space-group symbols: In this volume, as in *IT* A, the monoclinic space groups are listed for two settings. Nevertheless, the short symbol for the setting 'unique axis *b*' has been always used as the *standard* (short) HM symbol. It does not carry any information about the setting of the particular description. As in *IT* A, no other short symbols are used for monoclinic space groups and their subgroups in the present volume.

(2) 24 orthorhombic, tetragonal or cubic space-group types are listed with two different origins. In general, the origin is chosen at a point of highest site symmetry ('origin choice 1'); for exceptions see *IT* A, Section 8.3.1. If there are centres of inversion and if by this rule the origin is not at an inversion centre, then the space group is described once more with the origin at a centre of inversion ('origin choice 2').

(3) There are seven trigonal space groups with a rhombohedral lattice. These space groups are described in a hexagonal basis ('hexagonal axes') with a rhombohedrally centred hexagonal lattice as well as in a rhombohedral basis with a primitive lattice ('rhombohedral axes').

If there is a choice of setting for the space group $\mathcal{G}$, the chosen setting is indicated under the HM symbol in the headline. If a subgroup $\mathcal{H} < \mathcal{G}$ belongs to one of these 44 space-group types, its 'conventional setting' must be defined. The rules that are followed in this volume are explained in Section 2.1.2.5.

2.1.2.4. *Sequence of the subgroup and supergroup data*

As in the subgroup data of *IT* A, the sequence of the maximal subgroups is as follows: subgroups of the same kind are collected in a block. Each block has a heading. Compared with *IT* A, the blocks have been partly reorganized because in this volume *all* maximal isomorphic subgroups are listed, whereas in *IT* A only a few of them are described. In addition, the subgroups are described here in more detail.

The sequence of the subgroups within each block follows the value of the index; subgroups of lowest index are listed first. Subgroups having the same index are listed according to their lattice relations to the lattice of the original group $\mathcal{G}$, *cf.* Section 2.1.4.3.

[1] The clumsy terms 'plane-group type' and 'space-group type' are frequently abbreviated by the shorter terms 'plane group' and 'space group' in what follows, as is often done in crystallography. Occasionally, however, it is essential to distinguish the individual group from its 'type of groups'.

Subgroups with the same lattice relations are listed in decreasing order of space-group number.

Conjugate subgroups have the same index and the same space-group number. They are grouped together and connected by a brace on the left-hand side. Conjugate classes of maximal subgroups and their lengths are therefore easily recognized. In the series of maximal isomorphic subgroups, braces are inapplicable so here the conjugacy classes are stated explicitly.

The block designations are:

(1) In the block **I Maximal *translationengleiche* subgroups**, *all* maximal *translationengleiche* subgroups are listed, see Section 2.1.3. None of them are isomorphic.

(2) Under the heading **II Maximal *klassengleiche* subgroups**, all maximal *klassengleiche* subgroups are listed in up to three separate blocks, each of them marked by a bullet, •. Maximal non-isomorphic subgroups can only occur in the first two blocks, whereas maximal isomorphic subgroups are only found in the last two blocks.
   - **Loss of centring translations**. This block is described in Section 2.1.4.2 in more detail. Subgroups in this block are always non-isomorphic. The block is empty (and is then omitted) for space groups that are designated by an HM symbol starting with the letter *P*.
   - **Enlarged unit cell**. In this block, those maximal *klassengleiche* subgroups $\mathcal{H} < \mathcal{G}$ of index 2, 3 and 4 are listed for which the *conventional* unit cell of $\mathcal{H}$ is *larger* than that of $\mathcal{G}$, see Section 2.1.4.3. These subgroups may be non-isomorphic or isomorphic, see Section 2.1.5. Therefore, it may happen that a maximal isomorphic *klassengleiche* subgroup of index 2, 3 or 4 is listed twice: once here explicitly and once implicitly as a member of a series.
   - **Series of maximal isomorphic subgroups**. Maximal *klassengleiche* subgroups $\mathcal{H} < \mathcal{G}$ of indices 2, 3 and 4 may be isomorphic while those of index $i > 4$ are always isomorphic to $\mathcal{G}$. The total number of maximal *isomorphic klassengleiche* subgroups is infinite. These infinitely many subgroups cannot be described individually but only by a (small) number of infinite series. In each series, the individual subgroups are characterized by a few integer parameters, see Section 2.1.5.

(3) After the data for the subgroups, the data for the supergroups are listed. The data for minimal non-isomorphic supergroups are split into two main blocks with the headings
I Minimal *translationengleiche* supergroups and
II Minimal non-isomorphic *klassengleiche* supergroups.

(4) The latter block is split into the listings
• **Additional centring translations** and
• **Decreased unit cell**.

(5) Minimal isomorphic supergroups are not listed because they can be read immediately from the data for the maximal isomorphic subgroups.

For details, see Section 2.1.6.

2.1.2.5. *Special rules for the setting of the subgroups*

The multiple listing of 44 space-group types has implications for the subgroup tables. If a subgroup $\mathcal{H}$ belongs to one of these types, its 'conventional setting' must be defined. In many cases there is a natural choice; sometimes, however, such a choice does not exist, and the appropriate conventions have to be stated.

The three reasons for listing a space group twice will be discussed in this section, *cf.* Section 2.1.2.3.

2.1.2.5.1. *Monoclinic subgroups*

Rules:

(*a*) If the monoclinic axis of $\mathcal{H}$ is the *b* or *c* axis of the basis of $\mathcal{G}$, then the setting of $\mathcal{H}$ is also 'unique axis *b*' or 'unique axis *c*'. In particular, if $\mathcal{G}$ is monoclinic, then the settings of $\mathcal{G}$ and $\mathcal{H}$ agree.

(*b*) If the monoclinic axis of $\mathcal{H}$ is neither *b* nor *c* in the basis of $\mathcal{G}$, then for $\mathcal{H}$ the setting 'unique axis *b*' is chosen.

(*c*) The cell choice is always 'cell choice 1' with the symbols *C* and *c* for unique axis *b*, and *A* and *a* for unique axis *c*.

Remarks (see also the following examples):

Rule (*a*) is valid for the many cases where the setting of $\mathcal{H}$ is 'inherited' from $\mathcal{G}$. In particular, this always holds for isomorphic subgroups.

Rule (*b*) is applied if $\mathcal{G}$ is orthorhombic and the monoclinic axis of $\mathcal{H}$ is the *a* axis of $\mathcal{G}$ and if $\mathcal{H}$ is a monoclinic subgroup of a trigonal group. Rule (*b*) is not natural, but specifies a preference for the setting 'unique axis *b*'. This seems to be justified because the setting 'unique axis *b*' is used more frequently in crystallographic papers and the standard short HM symbol is also referred to it.

Rule (*c*) implies a choice of that cell which is most explicitly described in the tables of *IT* A. By this choice, the centring type and the glide vector are fixed to the conventional values of 'cell choice 1'.

The necessary adjustment is performed through a coordinate transformation, *i.e.* by a change of the basis and by an origin shift, see Section 2.1.3.3.

Example 2.1.2.5.1.

$\mathcal{G} = P12/m1$, No. 10; unique axis *b*.

II Maximal *klassengleiche* subgroups, Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}$, both subgroups $P12/a1$.

The monoclinic axis *b* is retained but the glide reflection *a* is converted into a glide reflection *c* ($P12/c1$ is the conventional HM symbol for cell choice 1).

[2] $\mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, all four subgroups $A12/m1$.

The monoclinic axis *b* is retained but the *A* centring is converted into the conventional *C* centring ($C12/m1$ is the conventional HM symbol for cell choice 1).

[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{c}' = 2\mathbf{c}$, both subgroups $B12/e1$. The monoclinic axis *b* is retained. The glide reflection is designated by '*e*' (simultaneous *c*- and *a*-glide reflection in the same plane perpendicular to **b**). The nonconventional *B* centring is converted into the conventional primitive setting *P*, by which the *e*-glide reflection also becomes a *c*-glide reflection.

Example 2.1.2.5.2.

$\mathcal{G} = P112/m$, No. 10; unique axis *c*.

II Maximal *klassengleiche* subgroups, Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}$, both subgroups $P112/a$.

The monoclinic axis *c* and the glide reflection *a* are retained because $P112/a$ is the conventional full HM symbol for unique axis *c*, cell choice 1.

[2] $\mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, all four subgroups $A112/m$.

The monoclinic axis *c* and the *A* centring are retained because $A112/m$ is the conventional full HM symbol for this setting.

[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$, both subgroups $C112/e$.

The monoclinic axis *c* is retained. The glide reflection is designated by '*e*' (simultaneous *a*- and *b*-glide reflection in the same plane perpendicular to **c**). The nonconventional *C* centring is converted into the conventional primitive setting *P*, by which the *e*-glide reflection also becomes an *a*-glide reflection.

Example 2.1.2.5.3.

$\mathcal{G} = Pban$, No. 50; origin choice 1.

I Maximal (monoclinic) ***translationengleiche* subgroups**

[2] $P112/n$: conventional unique axis *c*; nonconventional glide reflection *n*. The monoclinic axis *c* is retained but the glide reflection *n* is adjusted to a glide reflection *a* in order to conform to the conventional symbol $P112/a$ of cell choice 1.

[2] $P12/a1$: conventional unique axis *b*; nonconventional glide reflection *a*. The monoclinic axis *b* is retained but the glide reflection *a* is adjusted to a glide reflection *c* of the conventional symbol $P12/c1$, cell choice 1.

[2] $P2/b11$: nonconventional monoclinic unique axis *a*; nonconventional glide reflection *b*. The monoclinic axis *a* is transformed to the conventional unique axis *b*; the glide reflection *b* is adjusted to the conventional symbol $P12/c1$ of the setting unique axis *b*, cell choice 1.

2.1.2.5.2. *Subgroups with two origin choices*

Altogether, 24 orthorhombic, tetragonal and cubic space groups with inversions are listed twice in *IT* A. There are three kinds of possible ambiguities for such groups with two origin choices:

(*a*) Only the original group $\mathcal{G}$ is listed with two origin choices in *IT* A, $\mathcal{G}(1)$ and $\mathcal{G}(2)$, but the subgroup $\mathcal{H} < \mathcal{G}$ is listed with one origin. Then the matrix parts $\boldsymbol{P}$ for the transformations $(\boldsymbol{P}, \boldsymbol{p}_1)$ and $(\boldsymbol{P}, \boldsymbol{p}_2)$ of the coordinate systems of $\mathcal{G}(1)$ and $\mathcal{G}(2)$ to that of $\mathcal{H}$ are the same but the two columns of origin shift differ, namely $\boldsymbol{p}_1$ from $\mathcal{G}(1)$ to $\mathcal{H}$ and $\boldsymbol{p}_2$ from $\mathcal{G}(2)$ to $\mathcal{H}$. They are related to the shift $\boldsymbol{u}$ between the origins of $\mathcal{G}(1)$ and $\mathcal{G}(2)$. However, the transformations from both settings of the space group $\mathcal{G}$ to the setting of the space group $\mathcal{H}$ are not unique and there is some choice in the transformation matrix and the origin shift.

The transformation has been chosen such that

(i) it transforms the nonconventional description of the space group $\mathcal{H}$ to a conventional one;

(ii) the description of the crystal structure in the subgroup $\mathcal{H}$ is similar to that in the supergroup $\mathcal{G}$.

If it is not possible to achieve the latter aim, a transformation with simple matrix and column parts has been chosen which fulfils the first condition.

Example 2.1.2.5.4.

$\mathcal{G} = Pban$, No. 50, origin choice 1 and origin choice 2.

I Maximal *translationengleiche* subgroups

There are seven maximal *t*-subgroups of *Pban*, No. 50, four of which are orthorhombic, $\mathcal{H} = Pba2$, $Pb2n$, $P2an$ and $P222$, and three of which are monoclinic, $\mathcal{H} = P112/n$, $P12/a1$ and $P2/b11$. In the orthorhombic subgroups, the centres of inversion of $\mathcal{G}$ are lost but at least one kind of twofold axis is retained. Therefore, no origin shift for $\mathcal{H}$ is necessary from the setting 'origin choice 1' of $\mathcal{G}(1)$, where the origin is placed at the intersection of the three twofold axes. For the column part of the transformation $(\boldsymbol{P}, \boldsymbol{p}_1)$, $\boldsymbol{p}_1 = \boldsymbol{o}$ holds. For the monoclinic maximal *t*-subgroups of *Pban* the origin is shifted from the intersection of the three twofold axes in $\mathcal{G}(1)$ to an inversion centre of $\mathcal{H}$.

On the other hand, the origin is situated on an inversion centre for origin choice 2 of $\mathcal{G}(2)$, as is the origin in the conventional description of the three monoclinic maximal *t*-subgroups. For them the origin shift is $\boldsymbol{p}_2 = \boldsymbol{o}$, while there is a nonzero column $\boldsymbol{p}_2$ for the orthorhombic subgroups.

(*b*) Both $\mathcal{G}$ and its subgroup $\mathcal{H} < \mathcal{G}$ are listed with two origins. Then the origin choice of $\mathcal{H}$ is the same as that of $\mathcal{G}$. This rule always applies to isomorphic subgroups as well as in some other cases.

Example 2.1.2.5.5.

Maximal *k*-subgroups $\mathcal{H}$: *Pnnn*, No. 48, of the space group $\mathcal{G}$: *Pban*, No. 50. There are two such subgroups with the lattice relation $\mathbf{c}' = 2\mathbf{c}$. Both $\mathcal{G}$ and $\mathcal{H}$ are listed with two origins such that the origin choices of $\mathcal{G}$ and $\mathcal{H}$ are either the same or are strongly related.

(*c*) The group $\mathcal{G}$ is listed with one origin but the subgroup $\mathcal{H} < \mathcal{G}$ is listed with two origins. This situation is restricted to maximal *k*-subgroups with the only exception being $Ia\overline{3}d > I4_1/acd$, where there are three conjugate *t*-subgroups of index 3. In all cases the subgroup $\mathcal{H}$ is referred to origin choice 2. This rule is followed in the subgroup tables because it gives a better chance of retaining the origin of $\mathcal{G}$ in $\mathcal{H}$. If there are two origin choices for $\mathcal{H}$, then $\mathcal{H}$ has inversions and these are also elements of the supergroup $\mathcal{G}$. The (unique) origin of $\mathcal{G}$ is placed on one of the inversion centres. For origin choice 2 in $\mathcal{H}$, the origin of $\mathcal{H}$ may agree with that of $\mathcal{G}$, although this is not guaranteed. In addition, origin choice 2 is often preferred in structure determinations.

Example 2.1.2.5.6.

Maximal *k*-subgroups of *Pccm*, No. 49. In the block

• **Enlarged unit cell**, [2] $\mathbf{a}' = 2\mathbf{a}$

one finds two subgroups *Pcna* (50, *Pban*). One of them has the origin of $\mathcal{G}$, the origin of the other subgroup is shifted by $\frac{1}{2}, 0, 0$ and is placed on one of the inversion centres of $\mathcal{G}$ that is removed from the first subgroup. The analogous situation is found in the block [2] $\mathbf{b}' = 2\mathbf{b}$, where the two subgroups of space-group type *Pncb* (50, *Pban*) show the analogous relation. In the next block, [2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, the four subgroups *Ccce* (68) behave similarly.

For $\mathcal{G}$ = *Pmma*, No. 51, the same holds for the two subgroups of the type *Pmmn* (59) in the block [2] $\mathbf{b}' = 2\mathbf{b}$.

On the other hand, for $\mathcal{G}$ = *Immm*, No. 71, in the block 'Loss of centring translations' three subgroups of type *Pmmn* (59) and one of type *Pnnn* (48) are listed. All of them need an origin shift of $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ because they have lost the inversion centres of the origin of $\mathcal{G}$.

2.1.2.5.3. *Space groups with a rhombohedral lattice*

The seven trigonal space groups with a rhombohedral lattice are often called *rhombohedral space groups*. Their HM symbols begin with the lattice letter *R* and they are listed with both hexagonal axes and rhombohedral axes.

Rules:

(*a*) A rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is listed in the same setting as $\mathcal{G}$: if $\mathcal{G}$ is referred to hexagonal axes, so is $\mathcal{H}$; if $\mathcal{G}$ is referred to rhombohedral axes, so is $\mathcal{H}$.

(*b*) If $\mathcal{G}$ is a non-rhombohedral trigonal or a cubic space group, then a rhombohedral subgroup $\mathcal{H} < \mathcal{G}$ is always referred to hexagonal axes.

(*c*) A non-rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is referred to its standard setting.

Remarks:

Rule (*a*) provides a clear definition, in particular for the axes of isomorphic subgroups.

Rule (*b*) has been followed in the subgroup tables because the rhombohedral setting is rarely used in crystallography.

Rule (*c*) implies that monoclinic subgroups of rhombohedral space groups are referred to the setting 'unique axis *b*'.

There is a peculiarity caused by the two settings. The rhombohedral lattice appears to be centred in the hexagonal axes setting, whereas it is primitive in the rhombohedral axes setting. Therefore, there are trigonal subgroups of a rhombohedral space group $\mathcal{G}$ which are listed in the block 'Loss of centring translations' for the hexagonal axes setting of $\mathcal{G}$ but are listed in the block 'Enlarged unit cell' when $\mathcal{G}$ is referred to rhombohedral axes. Although unnecessary and not done for other space groups with primitive lattices, the line

• **Loss of centring translations** none

is listed for the rhombohedral axes setting.

Example 2.1.2.5.7.

$\mathcal{G} = R3$, No. 146. Maximal *klassengleiche* subgroups of index 2 and 3. Comparison of the subgroup data for the two settings of *R*3 shows that the subgroups $P3_2$ (145), $P3_1$ (144) and *P*3 (143) of index 3 appear in the block 'Loss of centring translations' for the hexagonal setting and in the block 'Enlarged unit cell' for the rhombohedral setting.

The sequence of the blocks has priority over the classification by increasing index. Therefore, in the setting 'hexagonal axes', the subgroups of index 3 precede the subgroup of index 2.

The complete general position is listed for the maximal *k*-subgroups of index 3 in the setting 'hexagonal axes'; only the generator is listed for rhombohedral axes.

2.1.3. I Maximal *translationengleiche* subgroups (*t*-subgroups)

2.1.3.1. *Introduction*

In this block, all maximal *t*-subgroups $\mathcal{H}$ of the plane groups and the space groups $\mathcal{G}$ are listed individually. Maximal *t*-subgroups are always non-isomorphic.

For the sequence of the subgroups, see Section 2.1.2.4. There are no lattice relations for *t*-subgroups because the lattice is retained. Therefore, the sequence is determined only by the rising value of the index and by the decreasing space-group number.

2.1.3.2. *A description in close analogy with IT A*

The listing is similar to that of *IT* A and presents on one line the following information for each subgroup $\mathcal{H}$:

[*i*] HMS1 (No., HMS2) sequence matrix shift

Conjugate subgroups are listed together and are connected by a left brace.

The symbols have the following meaning:

[i]	index of $\mathcal{H}$ in $\mathcal{G}$;
HMS1	HM symbol of $\mathcal{H}$ referred to the coordinate system and setting of $\mathcal{G}$. This symbol may be nonconventional;
No.	space-group No. of $\mathcal{H}$;
HMS2	conventional HM symbol of $\mathcal{H}$ if HMS1 is not a conventional HM symbol;
sequence	sequence of numbers; the numbers refer to those coordinate triplets of the general position of $\mathcal{G}$ that are retained in $\mathcal{H}$, *cf. Remarks*; for general position *cf.* Section 2.1.2.2.2;
matrix	matrix part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3;
shift	column part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3.

Remarks:

In the sequence column for space groups with centred lattices, the abbreviation '(numbers)+' means that the coordinate triplets specified by 'numbers' are to be taken plus those obtained by adding each of the centring translations, see the comments following Examples 2.1.3.2.1 and 2.1.3.2.2.

The symbol HMS2 is omitted if HMS1 is a conventional HM symbol.

The following deviations from the listing of *IT* A are introduced in these tables:

No.: the space-group No. of $\mathcal{H}$ is added.

HMS2: In order to specify the setting clearly, the *full* HM symbol is listed for monoclinic subgroups, not the standard (short) HM symbol as in *IT* A.

matrix, shift: These entries contain information on the transformation of $\mathcal{H}$ from the setting of $\mathcal{G}$ to the standard setting of $\mathcal{H}$. They are explained in Section 2.1.3.3.

The description of the subgroups can be explained by the following four examples.

Example 2.1.3.2.1.
$\mathcal{G}$: $C1m1$, No. 8, UNIQUE AXIS b

I Maximal *translationengleiche* subgroups

[2] $C1$ (1, $P1$)   1+

Comments:

HMS1: $C1$ is not a conventional HM symbol. Therefore, the conventional symbol $P1$ is added as HMS2 after the space-group number 1 of $\mathcal{H}$.

sequence: '1+' means x, y, z; $x+\frac{1}{2}, y+\frac{1}{2}, z$.

Example 2.1.3.2.2.
$\mathcal{G}$: $Fdd2$, No. 43

I Maximal *translationengleiche* subgroups

...

[2] $F112$ (5, $A112$)   (1; 2)+

Comments:

HMS1: $F112$ is not a conventional HM symbol; therefore, the conventional symbol $A112$ is added to the space-group No. 5 as HMS2. The setting unique axis c is inherited from $\mathcal{G}$.

sequence: (1, 2)+ means:

x, y, z; $x, y+\frac{1}{2}, z+\frac{1}{2}$; $x+\frac{1}{2}, y, z+\frac{1}{2}$; $x+\frac{1}{2}, y+\frac{1}{2}, z$;
$\bar{x}, \bar{y}, z$; $\bar{x}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$; $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$; $\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$;

Example 2.1.3.2.3.
$\mathcal{G}$: $P4_2/nmc = P4_2/n\,2_1/m\,2/c$, No. 137, ORIGIN CHOICE 2

I Maximal *translationengleiche* subgroups

...

[2] $P2/n\,2_1/m\,1$ (59, $Pmmn$)   1; 2; 5; 6; 9; 10; 13; 14

Comments:

HMS1: The sequence in the HM symbol for a tetragonal space group is **c**, **a**, **a** − **b**. From the parts $4_2/n$, $2_1/m$ and $2/c$ of the full HM symbol of $\mathcal{G}$, only $2/n$, $2_1/m$ and 1 remain in $\mathcal{H}$. Therefore, HMS1 is $P2/n\,2_1/m\,1$, and the conventional symbol $Pmmn$ is added as HMS2.

No.: The space-group number of $\mathcal{H}$ is 59. The setting origin choice 2 of $\mathcal{H}$ is inherited from $\mathcal{G}$.

sequence: The coordinate triplets of $\mathcal{G}$ retained in $\mathcal{H}$ are: (1) x, y, z; (2) $\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$; (5) $\bar{x}, y+\frac{1}{2}, \bar{z}$; (6) $x+\frac{1}{2}, \bar{y}, \bar{z}$; (9) $\bar{x}, \bar{y}, \bar{z}$; *etc.*

Example 2.1.3.2.4.
$\mathcal{G}$: $P3_112$, No. 151

I Maximal *translationengleiche* subgroups

[2] $P3_111$ (144, $P3_1$)	1; 2; 3		
⎧ [3] $P112$ (5, $C121$)	1; 6	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	
⎨ [3] $P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	0, 0, 1/3
⎩ [3] $P112$ (5, $C121$)	1; 5	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	0, 0, 2/3

Comments:

brace: The brace on the left-hand side connects the three conjugate monoclinic subgroups.

HMS1: $P112$ is not the conventional HM symbol for unique axis c but the constituent '2' of the nonconventional HM symbol refers to the directions $-2\mathbf{a}-\mathbf{b}$, $\mathbf{a}-\mathbf{b}$ and $\mathbf{a}+2\mathbf{b}$, in the hexagonal basis. According to the rules of Section 2.1.2.5, the standard setting is unique axis b, as expressed by the HM symbol $C121$.

HMS2: Note that the conventional monoclinic cell is centred.

matrix, shift: The entries in the columns 'matrix' and 'shift' are explained in the following Section 2.1.3.3 and evaluated in Example 2.1.3.3.2.

2.1.3.3. *Basis transformation and origin shift*

Each t-subgroup $\mathcal{H} < \mathcal{G}$ is defined by its representatives, listed under 'sequence' by numbers each of which designates an element of $\mathcal{G}$. These elements form the general position of $\mathcal{H}$. They are taken from the general position of $\mathcal{G}$ and, therefore, are referred to the coordinate system of $\mathcal{G}$. In the general position of $\mathcal{H}$, however, its elements are referred to the coordinate system of $\mathcal{H}$. In order to allow the transfer of the data from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$, the tools for this transformation are provided in the columns 'matrix' and 'shift' of the subgroup tables. The designation of the quantities is that of *IT* A Part 5 and is repeated here for convenience.

In the following, columns and rows are designated by boldface italic lower-case letters. Point coordinates $\boldsymbol{x}, \boldsymbol{x}'$, translation parts $\boldsymbol{w}$, $\boldsymbol{w}'$ of the symmetry operations and shifts $\boldsymbol{p}$, $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$ are represented by columns. The sets of basis vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (\boldsymbol{a})^{\mathrm{T}}$ and $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\boldsymbol{a}')^{\mathrm{T}}$ are represented by rows [indicated by $(\ldots)^{\mathrm{T}}$, which means 'transposed']. The quantities with unprimed symbols are referred to the coordinate system of $\mathcal{G}$, those with primes are referred to the coordinate system of $\mathcal{H}$.

The following columns will be used ($\boldsymbol{w}'$ is analogous to $\boldsymbol{w}$):

$$\boldsymbol{w}=\begin{pmatrix} w_1\\ w_2\\ w_3\end{pmatrix};\quad \boldsymbol{x}=\begin{pmatrix} x\\ y\\ z\end{pmatrix};\quad \boldsymbol{x}'=\begin{pmatrix} x'\\ y'\\ z'\end{pmatrix};\quad \boldsymbol{p}=\begin{pmatrix} p_1\\ p_2\\ p_3\end{pmatrix};\quad \boldsymbol{q}=\begin{pmatrix} q_1\\ q_2\\ q_3\end{pmatrix}.$$

The (3×3) matrices $\boldsymbol{W}$ and $\boldsymbol{W}'$ of the symmetry operations, as well as the matrix $\boldsymbol{P}$ for a change of basis and its inverse $\boldsymbol{Q}=\boldsymbol{P}^{-1}$, are designated by boldface italic upper-case letters ($\boldsymbol{W}'$ is analogous to $\boldsymbol{W}$):

$$\boldsymbol{W}=\begin{pmatrix} W_{11}\, W_{12}\, W_{13}\\ W_{21}\, W_{22}\, W_{23}\\ W_{31}\, W_{32}\, W_{33}\end{pmatrix};\ \boldsymbol{P}=\begin{pmatrix} P_{11}\, P_{12}\, P_{13}\\ P_{21}\, P_{22}\, P_{23}\\ P_{31}\, P_{32}\, P_{33}\end{pmatrix};\ \boldsymbol{Q}=\begin{pmatrix} Q_{11}\, Q_{12}\, Q_{13}\\ Q_{21}\, Q_{22}\, Q_{23}\\ Q_{31}\, Q_{32}\, Q_{33}\end{pmatrix}.$$

Let $\mathbf{a},\mathbf{b},\mathbf{c} = (\boldsymbol{a})^{\mathrm{T}}$ be the row of basis vectors of $\mathcal{G}$ and $\mathbf{a}',\mathbf{b}',\mathbf{c}' = (\boldsymbol{a}')^{\mathrm{T}}$ the basis of $\mathcal{H}$, then the basis $(\boldsymbol{a}')^{\mathrm{T}}$ is expressed in the basis $(\boldsymbol{a})^{\mathrm{T}}$ by the system of equations[2]

$$\begin{aligned}\mathbf{a}' &= P_{11}\,\mathbf{a}+P_{21}\,\mathbf{b}+P_{31}\,\mathbf{c}\\ \mathbf{b}' &= P_{12}\,\mathbf{a}+P_{22}\,\mathbf{b}+P_{32}\,\mathbf{c}\\ \mathbf{c}' &= P_{13}\,\mathbf{a}+P_{23}\,\mathbf{b}+P_{33}\,\mathbf{c}\end{aligned}\qquad (2.1.3.1)$$

or

$$(\mathbf{a}',\mathbf{b}',\mathbf{c}')^{\mathrm{T}} = (\mathbf{a},\mathbf{b},\mathbf{c})^{\mathrm{T}}\begin{pmatrix} P_{11}\, P_{12}\, P_{13}\\ P_{21}\, P_{22}\, P_{23}\\ P_{31}\, P_{32}\, P_{33}\end{pmatrix}. \qquad (2.1.3.2)$$

In matrix notation, this is

$$(\boldsymbol{a}')^{\mathrm{T}} = (\boldsymbol{a})^{\mathrm{T}}\boldsymbol{P}. \qquad (2.1.3.3)$$

The column $\boldsymbol{p}$ of coordinates of the origin O' of $\mathcal{H}$ is referred to the coordinate system of $\mathcal{G}$ and is called the *origin shift*. The matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$ describes the transformation from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$, for details, *cf.* *IT* A, Part 5. Therefore, $\boldsymbol{P}$ and $\boldsymbol{p}$ are chosen in the subgroup tables in the columns 'matrix' and 'shift', *cf.* Section 2.1.3.2. The column 'matrix' is empty if there is no change of basis, *i.e.* if $\boldsymbol{P}$ is the unit matrix $\boldsymbol{I}$. The column 'shift' is empty if there is no origin shift, *i.e.* if $\boldsymbol{p}$ is the column $\boldsymbol{o}$ consisting of zeroes only.

A change of the coordinate system, described by the matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$, changes the point coordinates from the column $\boldsymbol{x}$ to the column $\boldsymbol{x}'$. The formulae for this change do not contain the pair $(\boldsymbol{P},\boldsymbol{p})$ itself, but the related pair $(\boldsymbol{Q},\ \boldsymbol{q}) = (\boldsymbol{P}^{-1},\ -\boldsymbol{P}^{-1}\boldsymbol{p})$:

$$\boldsymbol{x}' = \boldsymbol{Q}\boldsymbol{x}+\boldsymbol{q} = \boldsymbol{P}^{-1}\boldsymbol{x}-\boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{x}-\boldsymbol{p}). \qquad (2.1.3.4)$$

Not only the point coordinates but also the matrix–column pairs for the symmetry operations are changed by a change of the coordinate system. A symmetry operation W is described in the coordinate system of $\mathcal{G}$ by the system of equations

$$\begin{aligned}\tilde{x} &= W_{11}\,x+W_{12}\,y+W_{13}\,z+w_1\\ \tilde{y} &= W_{21}\,x+W_{22}\,y+W_{23}\,z+w_2\\ \tilde{z} &= W_{31}\,x+W_{32}\,y+W_{33}\,z+w_3,\end{aligned}\qquad (2.1.3.5)$$

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x}+\boldsymbol{w} = (\boldsymbol{W},\boldsymbol{w})\,\boldsymbol{x}, \qquad (2.1.3.6)$$

i.e. by the matrix–column pair $(\boldsymbol{W},\boldsymbol{w})$. The symmetry operation W will be described in the coordinate system of the subgroup $\mathcal{H}$ by the equation

$$\tilde{\boldsymbol{x}}' = \boldsymbol{W}'\boldsymbol{x}'+\boldsymbol{w}' = (\boldsymbol{W}',\ \boldsymbol{w}')\,\boldsymbol{x}', \qquad (2.1.3.7)$$

and thus by the pair $(\boldsymbol{W}',\ \boldsymbol{w}')$. This pair can be calculated from the pair $(\boldsymbol{W},\ \boldsymbol{w})$ by solving the equations

$$\boldsymbol{W}' = \boldsymbol{Q}\,\boldsymbol{W}\boldsymbol{P} = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \qquad (2.1.3.8)$$

and

$$\boldsymbol{w}' = \boldsymbol{q}+\boldsymbol{Q}\boldsymbol{w}+\boldsymbol{Q}\boldsymbol{W}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{w}+\boldsymbol{W}\boldsymbol{p}-\boldsymbol{p}) = \boldsymbol{P}^{-1}(\boldsymbol{w}+(\boldsymbol{W}-\boldsymbol{I})\boldsymbol{p}). \qquad (2.1.3.9)$$

Example 2.1.3.3.1.

Consider the data listed for the *t*-subgroups of $Pmn2_1$, No. 31:

Index	HM & No.	sequence	matrix	shift
[2]	$P1n1$ (7, $P1c1$)	1; 3	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2]	$Pm11$ (6, $P1m1$)	1; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2]	$P112_1$ (4)	1; 2		1/4, 0, 0

This means that the matrices and origin shifts are

(1) $\boldsymbol{P}_1 = \begin{pmatrix} 0 & 0 & \bar{1}\\ 0 & 1 & 0\\ 1 & 0 & \bar{1}\end{pmatrix};\ \boldsymbol{P}_2 = \begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{pmatrix};\ \boldsymbol{P}_3 = \begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$

(2) $\boldsymbol{p}_1 = \begin{pmatrix} 0\\ 0\\ 0\end{pmatrix},\ \boldsymbol{p}_2 = \begin{pmatrix} 0\\ 0\\ 0\end{pmatrix},\ \boldsymbol{p}_3 = \begin{pmatrix} \frac{1}{4}\\ 0\\ 0\end{pmatrix}.$

(3) The first subgroup is monoclinic, the symmetry direction is the b axis, which is standard. However, the glide direction $\frac{1}{2}(\mathbf{a}+\mathbf{c})$ is nonconventional. Therefore, the basis of $\mathcal{G}$ is transformed to a basis of the subgroup $\mathcal{H}$ such that the b axis is retained, the glide direction becomes the c' axis and the a' axis is chosen such that the basis is a right-handed one, the angle $\beta' \geq 90°$ and the transformation matrix $\boldsymbol{P}$ is simple. This is done by the chosen matrix $\boldsymbol{P}_1$. The origin shift is the $\boldsymbol{o}$ column.
With equations (2.1.3.8) and (2.1.3.9), one obtains for the glide reflection $x,\bar{y},z-\frac{1}{2}$, which is $x,\bar{y},z+\frac{1}{2}$ after standardization by $0 \leq w_j < 1$.

(4) For the second monoclinic subgroup, the symmetry direction is the (nonconventional) a axis. The rules of Section 2.1.2.5 require a change to the setting 'unique axis b'. A cyclic permutation of the basis vectors is the simplest way to achieve this. The reflection $\bar{x},y,z$ is now described by $x,\bar{y},z$. Again there is no origin shift.

(5) The third monoclinic subgroup is in the conventional setting 'unique axis c', but the origin must be shifted onto the 2_1 screw axis. This is achieved by applying equation (2.1.3.9) with $\boldsymbol{p}_3$, which changes $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ of $Pmn2_1$ to $\bar{x},\bar{y},z+\frac{1}{2}$ of $P112_1$.

Example 2.1.3.3.2.

Evaluation of the *t*-subgroup data of the space group $P3_112$, No. 151, started in Example 2.1.3.2.4. The evaluation is now continued with the columns 'sequence', 'matrix' and 'shift'. They are used for the transformation of the elements of $\mathcal{H}$ to their conventional form. Only the monoclinic *t*-subgroups are of interest here because the trigonal subgroup is already in the standard setting.

[2] The system of equations (2.1.3.1) is similar but not identical to the system of equations (2.1.3.5), which describes a symmetry operation W by the matrix $\boldsymbol{W}$ and the column $\boldsymbol{w}$. Both $\boldsymbol{W}$ and $\boldsymbol{w}$ are listed as the general position in the space-group tables of *IT* A, *cf.* Part 5 and Chapter 11.2 of *IT* A. The essential difference is that in equation (2.1.3.6) the matrix $\boldsymbol{W}$ is multiplied by the column $\boldsymbol{x}$ from the *right-hand* side whereas in equation (2.1.3.3) the matrix $\boldsymbol{P}$ is multiplied by the row $(\boldsymbol{a})^{\mathrm{T}}$ from the *left-hand* side. Therefore, the running index in $\boldsymbol{W}$ is the second one, whereas in $\boldsymbol{P}$ it is the first one.

One takes from the tables of subgroups in Chapter 2.3

Index	HM & No.	sequence	matrix	shift
[3]	$P112$ (5, $C121$)	1; 6	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	
[3]	$P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	0, 0, 1/3
[3]	$P112$ (5, $C121$)	1; 5	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	0, 0, 2/3

Designating the three matrices by $\boldsymbol{P}_6, \boldsymbol{P}_4, \boldsymbol{P}_5$, one obtains

$$\boldsymbol{P}_6 = \begin{pmatrix} 0 & -2 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; \boldsymbol{P}_4 = \begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; \boldsymbol{P}_5 = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with the corresponding inverse matrices

$$\boldsymbol{Q}_6 = \begin{pmatrix} -\frac{1}{2} & 1 & 0 \\ -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; \boldsymbol{Q}_4 = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; \boldsymbol{Q}_5 = \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the origin shifts

$$\boldsymbol{p}_6 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \; \boldsymbol{p}_4 = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} \end{pmatrix}, \; \boldsymbol{p}_5 = \begin{pmatrix} 0 \\ 0 \\ \frac{2}{3} \end{pmatrix}.$$

For the three new bases this means

$$\mathbf{a}'_6 = \mathbf{b}, \; \mathbf{b}'_6 = -2\mathbf{a} - \mathbf{b}, \; \mathbf{c}'_6 = \mathbf{c}$$
$$\mathbf{a}'_4 = -\mathbf{a} - \mathbf{b}, \; \mathbf{b}'_4 = \mathbf{a} - \mathbf{b}, \; \mathbf{c}'_4 = \mathbf{c} \text{ and}$$
$$\mathbf{a}'_5 = \mathbf{a}, \; \mathbf{b}'_5 = \mathbf{a} + 2\mathbf{b}, \; \mathbf{c}'_5 = \mathbf{c}.$$

All these bases span ortho-hexagonal cells with twice the volume of the original hexagonal cell because for the matrices $\det(\boldsymbol{P}_i) = 2$ holds.
In the general position of $\mathcal{G} = P3_112$, No.151, one finds

$$(1)\; x, y, z; \;\; (4)\; \bar{y}, \bar{x}, \bar{z} + \tfrac{2}{3}; \;\; (5)\; \bar{x} + y, y, \bar{z} + \tfrac{1}{3}; \;\; (6)\; x, x - y, \bar{z}.$$

These entries represent the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$:

$$(1) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4) \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{2}{3} \end{pmatrix};$$

$$(5) \begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} \end{pmatrix}; \quad (6) \begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Application of equations (2.1.3.8) on the matrices $\boldsymbol{W}_k$ and (2.1.3.9) on the columns $\boldsymbol{w}_k$ of the matrix–column pairs results in

$$\boldsymbol{W}'_4 = \boldsymbol{W}'_5 = \boldsymbol{W}'_6 = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}; \; \boldsymbol{w}'_4 = \boldsymbol{w}'_6 = \boldsymbol{o}; \; \boldsymbol{w}'_5 = \begin{pmatrix} 0 \\ 0 \\ \bar{1} \end{pmatrix}.$$

All translation vectors of $\mathcal{G}$ are retained in the subgroups but the volume of the cells is doubled. Therefore, there must be centring-translation vectors in the new cells. For example, the application of equation (2.1.3.9) with $(\boldsymbol{P}_6, \boldsymbol{p}_6)$ to the translation of $\mathcal{G}$ with the vector $-\mathbf{a}$, *i.e.* $\boldsymbol{w} = -(1, 0, 0)$, results in the column $\boldsymbol{w}' = (\frac{1}{2}, \frac{1}{2}, 0)$, *i.e.* the centring translation $\frac{1}{2}(\mathbf{a}' + \mathbf{b}')$ of the subgroup. Either by calculation or, more easily, from a small sketch one sees that the vectors $-\mathbf{b}$ for $\boldsymbol{P}_4$, $\mathbf{a} + \mathbf{b}$ for $\boldsymbol{P}_5$ (and $-\mathbf{a}$ for $\boldsymbol{P}_6$) correspond to the cell-centring translation vectors of the subgroup cells.

Comments:

This example reveals that the conjugation of conjugate subgroups does not necessarily imply the conjugation of the representatives of these subgroups in the general positions of *IT* A. The three monoclinic subgroups $C121$ in this example are conjugate in the group $\mathcal{G}$ by the 3_1 screw rotation. Conjugation of the representative (4) by the 3_1 screw rotation of $\mathcal{G}$ results in the representative (5) with the column $\boldsymbol{w}_5 = 0, 0, \frac{4}{3}$, which is not exactly the representative (5) but one of its translationally equivalent elements of $\mathcal{G}$ retained in $\mathcal{H}$.

2.1.4. II Maximal *klassengleiche* subgroups (*k*-subgroups)

2.1.4.1. *General description*

The listing of the maximal *klassengleiche* subgroups (maximal *k*-subgroups) $\mathcal{H}_j$ of the space group $\mathcal{G}$ is divided into the following three blocks for practical reasons:

• **Loss of centring translations**. Maximal subgroups $\mathcal{H}$ of this block have the same conventional unit cell as the original space group $\mathcal{G}$. They are always non-isomorphic and have index 2 for plane groups and index 2, 3 or 4 for space groups.

• **Enlarged unit cell**. Under this heading, maximal subgroups of index 2, 3 and 4 are listed for which the *conventional* unit cell has been enlarged. The block contains isomorphic *and* non-isomorphic subgroups with this property.

• **Series of maximal isomorphic subgroups**. In this block *all* maximal isomorphic subgroups of a space group $\mathcal{G}$ are listed in a small number of infinite series of subgroups with no restriction on the index, *cf.* Sections 2.1.2.4 and 2.1.5.

The description of the subgroups is the same within the same block but differs between the blocks. The partition into these blocks differs from the partition in *IT* A, where the three blocks are called ‘maximal non-isomorphic subgroups IIa’, ‘maximal non-isomorphic subgroups IIb’ and ‘maximal isomorphic subgroups of lowest index IIc’.

The kind of listing in the three blocks of this volume is discussed in Sections 2.1.4.2, 2.1.4.3 and 2.1.5 below.

2.1.4.2. *Loss of centring translations*

Consider a space group $\mathcal{G}$ with a centred lattice, *i.e.* a space group whose HM symbol does not start with the lattice letter P but with one of the letters A, B, C, F, I or R. The block contains those maximal subgroups of $\mathcal{G}$ which have fully or partly lost their centring translations and thus are not *t*-subgroups. The *conventional* unit cell is *not* changed.

Only in space groups with an F-centred lattice can the centring be partially lost, as is seen in the list of the space group $Fmmm$, No. 69. On the other hand, for $F23$, No. 196, the maximal subgroups $P23$, No. 195, or $P2_13$, No. 198, have lost all their centring translations.

For the block ‘Loss of centring translations’, the listing in this volume is the same as that for *t*-subgroups, *cf.* Section 2.1.3. The centring translations are listed explicitly where applicable, *e.g.* for space group $C2$, No. 5, unique axis b

$$[2]\;\; P12_11\;\; (4) \qquad 1; 2 + (\tfrac{1}{2}, \tfrac{1}{2}, 0) \qquad 1/4, 0, 0.$$

In this line, the representatives 1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$ of the general position are $x, y, z \quad \bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$.

The listing differs from that in *IT* A in only two points:

(1) the full HM symbol is taken as the conventional symbol for monoclinic space groups, whereas in *IT* A the short HM symbol is the conventional one;
(2) the information needed for the transformation of the data from the setting of the space group $\mathcal{G}$ to that of $\mathcal{H}$ is added. In this example, the matrix is the unit matrix and is not listed; the column of origin shift is $\frac{1}{4}, 0, 0$. This transformation is analogous to that of *t*-subgroups and is described in detail in Section 2.1.3.3.

The sequence of the subgroups in this block is one of decreasing space-group number of the subgroups.

2.1.4.3. *Enlarged unit cell*

Under the heading 'Enlarged unit cell', those maximal *k*-subgroups $\mathcal{H}$ are listed for which the conventional unit cell is enlarged relative to the unit cell of the original space group $\mathcal{G}$. *All* maximal *k*-subgroups with enlarged unit cell of index 2, 3 or 4 of the plane groups and of the space groups are listed *individually*. The listing is restricted to these indices because 4 is the highest index of a maximal *non-isomorphic* subgroup, and the number of these subgroups is finite. Maximal subgroups of higher indices are always isomorphic to $\mathcal{G}$ and their number is infinite.

The description of the subgroups with enlarged unit cell is more detailed than in *IT* A. In the block IIb of *IT* A, different maximal subgroups of the same space-group type with the same lattice relations are represented by the same entry. For example, the eight maximal subgroups of the type *Fmmm*, No. 69, of space group *Pmmm*, No. 47, are represented by one entry in *IT* A.

In the present volume, the description of the maximal subgroups in the block 'Enlarged unit cell' refers to each subgroup individually and contains for each of them a set of space-group generators and the transformation from the setting of the space group $\mathcal{G}$ to the conventional setting of the subgroup $\mathcal{H}$.

Some of the isomorphic subgroups listed in this block may also be found in *IT* A in the block 'Maximal isomorphic subgroups of lowest index IIc'.

Subgroups with the same lattice are collected in small blocks. The heading of each such block consists of the index of the subgroup and the lattice relations of the sublattice relative to the original lattice. Basis vectors that are not mentioned are not changed.

Example 2.1.4.3.1.

This example is taken from the table of space group $C222_1$, No. 20.

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$

$$\left\{\begin{array}{lll} C222_1\ (20)\ \langle 2;3\rangle & 3\mathbf{a},\mathbf{b},\mathbf{c} & \\ C222_1\ (20)\ \langle (2;3)+(2,0,0)\rangle & 3\mathbf{a},\mathbf{b},\mathbf{c} & 1,0,0 \\ C222_1\ (20)\ \langle (2;3)+(4,0,0)\rangle & 3\mathbf{a},\mathbf{b},\mathbf{c} & 2,0,0 \end{array}\right.$$

[3] $\mathbf{b}' = 3\mathbf{b}$

$$\left\{\begin{array}{lll} C222_1\ (20)\ \langle 2;3\rangle & \mathbf{a},3\mathbf{b},\mathbf{c} & \\ C222_1\ (20)\ \langle 3;2+(0,2,0)\rangle & \mathbf{a},3\mathbf{b},\mathbf{c} & 0,1,0 \\ C222_1\ (20)\ \langle 3;2+(0,4,0)\rangle & \mathbf{a},3\mathbf{b},\mathbf{c} & 0,2,0 \end{array}\right.$$

The entries mean:

Columns 1 and 2: HM symbol and space-group number of the subgroup; *cf.* Section 2.1.3.2.

Column 3: generators, here the pairs

$$\begin{array}{ll} \bar{x},\bar{y},z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \\ \bar{x}+2,\bar{y},z+\frac{1}{2}; & \bar{x}+2,y,\bar{z}+\frac{1}{2}; \\ \bar{x}+4,\bar{y},z+\frac{1}{2}; & \bar{x}+4,y,\bar{z}+\frac{1}{2}; \end{array}$$

$$\begin{array}{ll} \bar{x},\bar{y},z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \\ \bar{x},\bar{y}+2,z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \\ \bar{x},\bar{y}+4,z+\frac{1}{2}; & \bar{x},y,\bar{z}+\frac{1}{2}; \end{array}$$

for the six lines listed in the same order.

Column 4: basis vectors of $\mathcal{H}$ referred the basis vectors of $\mathcal{G}$. $3\mathbf{a},\mathbf{b},\mathbf{c}$ means $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$; $\mathbf{a},3\mathbf{b},\mathbf{c}$ means $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$.

Column 5: origin shifts, referred to the coordinate system of $\mathcal{G}$. These origin shifts by $\mathbf{o}$, $\mathbf{a}$ and $2\mathbf{a}$ for the first triplet of subgroups and $\mathbf{o}$, $\mathbf{b}$ and $2\mathbf{b}$ for the second triplet of subgroups are translations of $\mathcal{G}$. The subgroups of each triplet are conjugate, indicated by the left braces.

Often the lattice relations above the data describing the subgroups are the same as the basis vectors in column 4, as in this example. They differ in particular if the sublattice of $\mathcal{H}$ is non-conventionally centred. Examples are the *H*-centred subgroups of trigonal and hexagonal space groups.

The sequence of the subgroups is determined

(1) by the index of the subgroup such that the subgroups of lowest index are given first;
(2) within the same index by the kind of cell enlargement;
(3) within the same cell enlargement by the No. of the subgroup, such that the subgroup of highest space-group number is given first.

2.1.4.3.1. *Enlarged unit cell, index 2*

For sublattices with twice the volume of the unit cell, the sequence of the different cell enlargements is as follows:

(1) Triclinic space groups:
   - (i) $\mathbf{a}' = 2\mathbf{a}$,
   - (ii) $\mathbf{b}' = 2\mathbf{b}$,
   - (iii) $\mathbf{c}' = 2\mathbf{c}$,
   - (iv) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
   - (v) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
   - (vi) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
   - (vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.

(2) Monoclinic space groups:
   - (*a*) with *P* lattice, unique axis *b*:
     - (i) $\mathbf{b}' = 2\mathbf{b}$,
     - (ii) $\mathbf{c}' = 2\mathbf{c}$,
     - (iii) $\mathbf{a}' = 2\mathbf{a}$,
     - (iv) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
     - (v) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
     - (vi) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
     - (vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.
   - (*b*) with *P* lattice, unique axis *c*:
     - (i) $\mathbf{c}' = 2\mathbf{c}$,
     - (ii) $\mathbf{a}' = 2\mathbf{a}$,
     - (iii) $\mathbf{b}' = 2\mathbf{b}$,
     - (iv) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
     - (v) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
     - (vi) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
     - (vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.

(*c*) with *C* lattice, unique axis *b*: There are three sublattices of index 2 of a monoclinic *C* lattice. One has lost its centrings such that a *P* lattice with the same unit cell remains. The subgroups with this sublattice are listed under 'Loss of centring translations'. The block with the other two sublattices consists of $\mathbf{c}' = 2\mathbf{c}$, *C*-centring and *I*-centring. The sequence of the subgroups in this block is determined by the space-group number of the subgroup.

(*d*) with *A* lattice, unique axis *c*: There are three sublattices of index 2 of a monoclinic *A* lattice. One has lost its centrings such that a *P* lattice with the same unit cell remains. The subgroups with this sublattice are listed under 'Loss of centring translations'. The block with the other two sublattices consists of $\mathbf{a}' = 2\mathbf{a}$, *A*-centring and *I*-centring. The sequence of the subgroups in this block is determined by the No. of the subgroup.

(3) Orthorhombic space groups:

(*a*) Orthorhombic space groups with *P* lattice: Same sequence as for triclinic space groups.

(*b*) Orthorhombic space groups with *C* (or *A*) lattice: Same sequence as for monoclinic space groups with *C* (or *A*) lattice.

(*c*) Orthorhombic space groups with *I* and *F* lattice: There are no subgroups of index 2 with enlarged unit cell.

(4) Tetragonal space groups:

(*a*) Tetragonal space groups with *P* lattice:

(i) $\mathbf{c}' = 2\mathbf{c}$.

(ii) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$, *C*-centring. The conventional setting results in a *P* lattice.

(iii) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, *F*-centring. The conventional setting results in an *I* lattice.

(*b*) Tetragonal space groups with *I* lattice: There are no subgroups of index 2 with enlarged unit cell.

(5) For trigonal and hexagonal space groups, $\mathbf{c}' = 2\mathbf{c}$ holds.
For rhombohedral space groups referred to hexagonal axes, $\mathbf{a}' = -\mathbf{b},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = \mathbf{a}+\mathbf{b},\ \mathbf{b}' = -\mathbf{a},\ \mathbf{c}' = 2\mathbf{c}$ holds.
For rhombohedral space groups referred to rhombohedral axes, $\mathbf{a}' = \mathbf{a}+\mathbf{c},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = \mathbf{b}+\mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, *F*-centring holds.

(6) Only cubic space groups with a *P* lattice have subgroups of index 2 with enlarged unit cell. For their lattices the following always holds: $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, *F*-centring.

2.1.4.3.2. *Enlarged unit cell, index 3 or 4*

With a few exceptions for trigonal, hexagonal and cubic space groups, *k*-subgroups with enlarged unit cells and index 3 or 4 are isomorphic. To each of the listed sublattices belong either one or several conjugacy classes with three or four conjugate subgroups or one or several normal subgroups. Only the sublattices with the numbers (5)(*a*)(v), (5)(*b*)(i), (5)(*c*)(ii), (6)(iii) and (7)(i) have index 4, all others have index 3. The different cell enlargements are listed in the following sequence:

(1) Triclinic space groups:

(i) $\mathbf{a}' = 3\mathbf{a}$,
(ii) $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = \mathbf{a}+\mathbf{b}$,
(iii) $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}$,
(iv) $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = \mathbf{a}+\mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a}, \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$,
(vi) $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = \mathbf{a}+\mathbf{b}, \mathbf{c}' = \mathbf{a}+\mathbf{c}$,
(vii) $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}, \mathbf{c}' = \mathbf{a}+\mathbf{c}$,
(viii) $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = \mathbf{a}+\mathbf{b}, \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$,
(ix) $\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 2\mathbf{a}+\mathbf{b}, \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$,
(x) $\mathbf{b}' = 3\mathbf{b}$,
(xi) $\mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = \mathbf{b}+\mathbf{c}$,
(xii) $\mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 2\mathbf{b}+\mathbf{c}$,
(xiii) $\mathbf{c}' = 3\mathbf{c}$.

(2) Monoclinic space groups:

(*a*) Space groups $P121$, $P12_11$, $P1m1$, $P12/m1$, $P12_1/m1$ (unique axis *b*):

(i) $\mathbf{b}' = 3\mathbf{b}$,
(ii) $\mathbf{c}' = 3\mathbf{c}$,
(iii) $\mathbf{a}' = \mathbf{a}-\mathbf{c}, \mathbf{c}' = 3\mathbf{c}$,
(iv) $\mathbf{a}' = \mathbf{a}-2\mathbf{c}, \mathbf{c}' = 3\mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a}$.

(*b*) Space groups $P112$, $P112_1$, $P11m$, $P112/m$, $P112_1/m$ (unique axis *c*):

(i) $\mathbf{c}' = 3\mathbf{c}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$,
(iii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -\mathbf{a}+\mathbf{b}$,
(iv) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$,
(v) $\mathbf{b}' = 3\mathbf{b}$.

(*c*) Space groups $P1c1$, $P12/c1$, $P12_1/c1$ (unique axis *b*):

(i) $\mathbf{b}' = 3\mathbf{b}$,
(ii) $\mathbf{c}' = 3\mathbf{c}$,
(iii) $\mathbf{a}' = 3\mathbf{a}$,
(iv) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{c}' = -2\mathbf{a}+\mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{c}' = -4\mathbf{a}+\mathbf{c}$.

(*d*) Space groups $P11a$, $P112/a$, $P112_1/a$ (unique axis *c*):

(i) $\mathbf{c}' = 3\mathbf{c}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$,
(iii) $\mathbf{b}' = 3\mathbf{b}$,
(iv) $\mathbf{a}' = \mathbf{a}-2\mathbf{b},\ \mathbf{b}' = 3\mathbf{b}$,
(v) $\mathbf{a}' = \mathbf{a}-4\mathbf{b},\ \mathbf{b}' = 3\mathbf{b}$.

(*e*) All space groups with *C* lattice (unique axis *b*):

(i) $\mathbf{b}' = 3\mathbf{b}$,
(ii) $\mathbf{c}' = 3\mathbf{c}$,
(iii) $\mathbf{a}' = \mathbf{a}-2\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$,
(iv) $\mathbf{a}' = \mathbf{a}-4\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a}$.

(*f*) All space groups with *A* lattice (unique axis *c*):

(i) $\mathbf{c}' = 3\mathbf{c}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$,
(iii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$,
(iv) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -4\mathbf{a}+\mathbf{b}$,
(v) $\mathbf{b}' = 3\mathbf{b}$.

(3) Orthorhombic space groups:

(i) $\mathbf{a}' = 3\mathbf{a}$,
(ii) $\mathbf{b}' = 3\mathbf{b}$,
(iii) $\mathbf{c}' = 3\mathbf{c}$.

(4) Tetragonal space groups:

(i) $\mathbf{c}' = 3\mathbf{c}$.

(5) Trigonal space groups:

(*a*) Trigonal space groups with hexagonal *P* lattice:

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b},\ H$-centring,

(iii) $\mathbf{a}' = \mathbf{a} - \mathbf{b},\ \mathbf{b}' = \mathbf{a} + 2\mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$, *R* lattice,

(iv) $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}, \mathbf{b}' = -\mathbf{a} + \mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$, *R* lattice,

(v) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$.

(*b*) Trigonal space groups with rhombohedral *R* lattice and hexagonal axes:

(i) $\mathbf{a}' = -2\mathbf{b},\ \mathbf{b}' = 2\mathbf{a} + 2\mathbf{b}$.

(*c*) Trigonal space groups with rhombohedral *R* lattice and rhombohedral axes:

(i) $\mathbf{a}' = \mathbf{a} - \mathbf{b},\ \mathbf{b}' = \mathbf{b} - \mathbf{c},\ \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$,

(ii) $\mathbf{a}' = \mathbf{a} - \mathbf{b} + \mathbf{c},\ \mathbf{b}' = \mathbf{a} + \mathbf{b} - \mathbf{c},\ \mathbf{c}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}$.

(6) Hexagonal space groups:

(i) $\mathbf{c}' = 3\mathbf{c}$,

(ii) $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b},\ H$-centring,

(iii) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$.

(7) Cubic space groups with *P* lattice:

(i) $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$, *I* lattice.

2.1.5. Series of maximal isomorphic subgroups

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2.1.5.1. *General description*

Maximal subgroups of index higher than 4 have index p, p^2 or p^3, where p is prime, are necessarily isomorphic subgroups and are infinite in number. Only a few of them are listed in *IT* A in the block 'Maximal isomorphic subgroups of lowest index IIc'. Because of their infinite number, they cannot be listed individually, but are listed in this volume as members of series under the heading 'Series of maximal isomorphic subgroups'. In most of the series, the HM symbol for each isomorphic subgroup $\mathcal{H} < \mathcal{G}$ will be the same as that of $\mathcal{G}$. However, if $\mathcal{G}$ is an enantiomorphic space group, the HM symbol of $\mathcal{H}$ will be either that of $\mathcal{G}$ or that of its enantiomorphic partner.

Example 2.1.5.1.1.

Two of the four series of isomorphic subgroups of the space group $P4_1$, No. 76, are (the data on the generators are omitted):

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 2;\ p \equiv 3 \pmod 4$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	$P4_1$ (76)	$p > 4;\ p \equiv 1 \pmod 4$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$

On the other hand, the corresponding data for $P4_3$, No. 78, are

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 4;\ p \equiv 1 \pmod 4$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	$P4_1$ (76)	$p > 2;\ p \equiv 3 \pmod 4$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$

Note that in both tables the subgroups of the type $P4_3$, No. 78, are listed first because of the rules on the sequence of the subgroups.

If an isomorphic maximal subgroup of index $i \le 4$ is a member of a series, then it is listed twice: as a member of its series *and* individually under the heading 'Enlarged unit cell'.

Most isomorphic subgroups of index 3 are the first members of series but those of index 2 or 4 are rarely so. An example is the space group $P4_2$, No. 77, with isomorphic subgroups of index 2 (not in any series) and 3 (in a series); an exception is found in space group $P4$, No. 75, where the isomorphic subgroup for $\mathbf{c}' = 2\mathbf{c}$ is the first member of the series $[p]\ \mathbf{c}' = p\mathbf{c}$.

2.1.5.2. *Basis transformation*

The conventional basis of the unit cell of each isomorphic subgroup in the series has to be defined relative to the basis of the original space group. For this definition the prime p is frequently sufficient as a parameter.

Example 2.1.5.2.1.

The isomorphic subgroups of the space group $P4_222$, No. 93, can be described by two series with the bases of their members:

$[p]$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
$[p^2]$	$p\mathbf{a},\ p\mathbf{b},\ \mathbf{c}$.

In other cases, one or two positive integers, here called q and r, define the series and often the value of the prime p.

Example 2.1.5.2.2.

In space group $P\overline{6}$, No. 174, the series $q\mathbf{a} - r\mathbf{b},\ r\mathbf{a} + (q+r)\mathbf{b},\ \mathbf{c}$ is listed. The values of q and r have to be chosen such that while $q > 0,\ r > 0,\ p = q^2 + r^2 + qr$ and p is prime.

Example 2.1.5.2.3.

In the space group $P112_1/m$, No. 11, unique axis c, the series $p\mathbf{a},\ -q\mathbf{a} + \mathbf{b},\ \mathbf{c}$ is listed. Here p and q are independent and q may take the p values $0 \le q < p$ for each value of p.

2.1.5.3. *Origin shift*

Each of the sublattices discussed in Section 2.1.4.3.2 is common to a conjugacy class or belongs to a normal subgroup of a given series. The subgroups in a conjugacy class differ by the positions of their conventional origins relative to the origin of the space group $\mathcal{G}$. To define the origin of the conventional unit cell of each subgroup in a conjugacy class, one, two or three integers, called u, v or w in these tables, are necessary. For a series of subgroups of index p, p^2 or p^3 there are p, p^2 or p^3 conjugate subgroups, respectively. The positions of their origins are defined by the p or p^2 or p^3 permitted values of u or u, v or u, v, w, respectively.

Example 2.1.5.3.1.

The space group $\mathcal{G}$, $P\overline{4}2c$, No. 112, has two series of maximal isomorphic subgroups $\mathcal{H}$. For one of them the lattice relations are $[p^2]\ \mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$, listed as $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ for the transformation matrix. The index is p^2. For each value of p there exist exactly p^2 conjugate subgroups with origins in the points $u,\ v,\ 0$, where the parameters u and v run independently: $0 \le u < p$ and $0 \le v < p$.

In another type of series there is exactly one (normal) subgroup $\mathcal{H}$ for each index p; the location of its origin is always chosen at the origin $0, 0, 0$ of $\mathcal{G}$ and is thus not indicated as an origin shift.

Example 2.1.5.3.2.

Consider the space group $Pca2_1$, No. 29. Only one subgroup exists for each value of p in the series $\mathbf{a}, \mathbf{b}, p\mathbf{c}$. This is indicated in the tables by the statement 'no conjugate subgroups'.

2.1.5.4. *Generators*

The generators of the p (or p^2 or p^3) conjugate isomorphic subgroups $\mathcal{H}$ are obtained from those of $\mathcal{G}$ by adding translational components. These components are determined by the parameters p (or q and r, if relevant) and u (and v and w, if relevant).

Example 2.1.5.4.1.
Space group $P2_13$, No. 198.
In the series defined by the lattice relations $p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ and the origin shift u, v, w there exist exactly p^3 conjugate subgroups for each value of p. The generators of each subgroup are defined by the parameter p and the triplet u, v, w in combination with the generators (2), (3) and (5) of $\mathcal{G}$. Consider the subgroup characterized by the basis $7\mathbf{a}, 7\mathbf{b}, 7\mathbf{c}$ and by the origin shift $u = 3$, $v = 4$, $w = 6$. One obtains from the generator (2) $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$ of $\mathcal{G}$ the corresponding generator of $\mathcal{H}$ by adding the translation vector $(\frac{p}{2}-\frac{1}{2}+2u)\mathbf{a}+2v\mathbf{b}+(\frac{p}{2}-\frac{1}{2})\mathbf{c}$ to the translation vector $\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{c}$ of the generator (2) of $\mathcal{G}$ and obtains $\frac{19}{2}\,\mathbf{a}+8\mathbf{b}+\frac{7}{2}\,\mathbf{c}$, so that this generator of $\mathcal{H}$ is written $\bar{x}+\frac{19}{2}, \bar{y}+8, z+\frac{7}{2}$.

2.1.5.5. *Special series*

For most space groups, there is only one description of their series of the isomorphic subgroups. However, if a space group is described twice in *IT* A, then there are also two different descriptions of these series. This happens for monoclinic space groups with the settings unique axis b and unique axis c, for some orthorhombic, tetragonal and cubic space groups with origin choice 1 and origin choice 2 and for trigonal space groups with rhombohedral lattices with hexagonal axes and rhombohedral axes.

2.1.5.5.1. *Monoclinic space groups*

In the monoclinic space groups, the series in the listings 'unique axis b' and 'unique axis c' are closely related by a simple cyclic permutation of the axes a, b and c, see *IT* A, Section 2.2.16.

2.1.5.5.2. *Trigonal space groups with rhombohedral lattice*

In trigonal space groups with rhombohedral lattices, the series with hexagonal axes and with rhombohedral axes appear to be rather different. However, the 'rhombohedral' series are the exact transcript of the 'hexagonal' series by the same transformation formulae as are used for the different monoclinic settings. However, the transformation matrices $\boldsymbol{P}$ and $\boldsymbol{P}^{-1}$ in Part 5 of *IT* A are more complicated in this case.

Example 2.1.5.5.1.
Space group $R\bar{3}$, No. 148. The second series is described with hexagonal axes by the basis transformation $\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$, *i.e.* $\mathbf{a}'_{\rm hex} = \mathbf{a}_{\rm hex}$, $\mathbf{b}'_{\rm hex} = \mathbf{b}_{\rm hex}$, $\mathbf{c}'_{\rm hex} = p\,\mathbf{c}_{\rm hex}$, and the origin shift $0, 0, u$. We discuss the basis transformation first. It can be written

$$(\mathbf{a}'_{\rm hex})^{\rm T} = (\mathbf{a}_{\rm hex})^{\rm T}\boldsymbol{X} \tag{2.1.5.1}$$

in analogy to Part 5, *IT* A. Here $(\mathbf{a}_{\rm hex})^{\rm T}$ is the row of basis vectors of the conventional hexagonal basis. The matrix $\boldsymbol{X}$ is defined by

$$\boldsymbol{X} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & p \end{pmatrix}.$$

With rhombohedral axes, equation (2.1.5.1) would be written

$$(\mathbf{a}'_{\rm rh})^{\rm T} = (\mathbf{a}_{\rm rh})^{\rm T}\boldsymbol{Y}, \tag{2.1.5.2}$$

with the matrix $\boldsymbol{Y}$ to be determined.
The transformation from hexagonal to rhombohedral axes is described by

$$(\mathbf{a}_{\rm rh})^{\rm T} = (\mathbf{a}_{\rm hex})^{\rm T}\boldsymbol{P}^{-1}, \tag{2.1.5.3}$$

where the matrices

$$\boldsymbol{P}^{-1} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \text{ and } \boldsymbol{P} = \begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$$

are listed in *IT* A, Table 5.1.3.1, see also Figs. 5.1.3.6 (*a*) and (*c*) in *IT* A.
Applying equations (2.1.5.3), (2.1.5.1) and (2.1.5.2), one gets

$$(\mathbf{a}'_{\rm rh})^{\rm T} = (\mathbf{a}'_{\rm hex})^{\rm T}\boldsymbol{P}^{-1} = (\mathbf{a}_{\rm hex})^{\rm T}\boldsymbol{X}\boldsymbol{P}^{-1} = (\mathbf{a}_{\rm rh})^{\rm T}\boldsymbol{Y} = (\mathbf{a}_{\rm hex})^{\rm T}\boldsymbol{P}^{-1}\boldsymbol{Y}. \tag{2.1.5.4}$$

From equation (2.1.5.4) it follows that

$$\boldsymbol{X}\boldsymbol{P}^{-1} = \boldsymbol{P}^{-1}\boldsymbol{Y} \text{ or } \boldsymbol{Y} = \boldsymbol{P}\boldsymbol{X}\boldsymbol{P}^{-1}. \tag{2.1.5.5}$$

One obtains $\boldsymbol{Y}$ from equation (2.1.5.5) by matrix multiplication,

$$\boldsymbol{Y} = \begin{pmatrix} \frac{p+2}{3} & \frac{p-1}{3} & \frac{p-1}{3} \\ \frac{p-1}{3} & \frac{p+2}{3} & \frac{p-1}{3} \\ \frac{p-1}{3} & \frac{p-1}{3} & \frac{p+2}{3} \end{pmatrix},$$

and from $\boldsymbol{Y}$ for the bases of the subgroups with rhombohedral axes

$$\mathbf{a}'_{\rm rh} = \tfrac{1}{3}[(p+2)\mathbf{a}_{\rm rh} + (p-1)\mathbf{b}_{\rm rh} + (p-1)\mathbf{c}_{\rm rh}],$$
$$\mathbf{b}'_{\rm rh} = \tfrac{1}{3}[(p-1)\mathbf{a}_{\rm rh} + (p+2)\mathbf{b}_{\rm rh} + (p-1)\mathbf{c}_{\rm rh}],$$
$$\mathbf{c}'_{\rm rh} = \tfrac{1}{3}[(p-1)\mathbf{a}_{\rm rh} + (p-1)\mathbf{b}_{\rm rh} + (p+2)\mathbf{c}_{\rm rh}].$$

The column of the origin shift $\boldsymbol{u}_{\rm hex} = 0, 0, u$ in hexagonal axes must be transformed by $\boldsymbol{u}_{\rm rh} = \boldsymbol{P}\,\boldsymbol{u}_{\rm hex}$. The result is the column $\boldsymbol{u}_{\rm rh} = u,\ u,\ u$ in rhombohedral axes.

2.1.5.5.3. *Space groups with two origin choices*

Space groups with two origin choices are always described in the same basis, but origin 1 is shifted relative to origin 2 by the shift vector $\mathbf{s}$. For most space groups with two origins, the appearance of the two series related by the origin shift is similar; there are only differences in the generators.

Example 2.1.5.5.2.
Consider the space group *Pnnn*, No. 48, in both origin choices and the corresponding series defined by $p\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and u, 0, 0. In origin choice 1, the generator (5) of $\mathcal{G}$ is described by the 'coordinates' $\bar{x}+\frac{1}{2}$, $\bar{y}+\frac{1}{2}$, $\bar{z}+\frac{1}{2}$. The translation part $(\frac{p}{2}-\frac{1}{2})\mathbf{a}$ of the third generator of $\mathcal{H}$ stems from the term $\frac{1}{2}$ in the first 'coordinate' of the generator (5) of $\mathcal{G}$. Because $(\frac{p}{2}-\frac{1}{2})\mathbf{a}$ must be a translation vector of $\mathcal{G}$, p is odd. Such a translation part is not found in the generators (2) and (3) of $\mathcal{H}$ because the term $\frac{1}{2}$ does not appear in the 'coordinates' of the corresponding generators of $\mathcal{G}$.
The situation is inverted in the description for origin choice 2. The translation term $(\frac{p}{2}-\frac{1}{2})\mathbf{a}$ appears in the first and second generator of $\mathcal{H}$ and not in the third one because the term $\frac{1}{2}$

occurs in the first 'coordinate' of the generators (2) and (3) of $\mathcal{G}$ but not in the generator (5).
The term $2u$ appears in both descriptions. It is introduced in order to adapt the generators to the origin shift u, 0, 0.

In other space groups described in two origin choices, surprisingly, the number of series is different for origin choice 1 and origin choice 2.

Example 2.1.5.5.3.
In the tetragonal space group $I4_1/amd$, No. 141, for origin choice 1 there is *one* series of maximal isomorphic subgroups of index p^2, p prime, with the bases $p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ and origin shifts u, v, 0. For origin choice 2, there are *two* series with the same bases $p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ but with the different origin shifts u, v, 0 and $\frac{1}{2}+u$, v, 0. What are the reasons for these results?
For origin choice 1, the term $\frac{1}{2}$ appears in the first and second 'coordinates' of all generators (2), (3), (5) and (9) of $\mathcal{G}$. This term $\frac{1}{2}$ is the cause of the translation vectors $(\frac{p}{2}-\frac{1}{2})\mathbf{a}$ and $(\frac{p}{2}-\frac{1}{2})\mathbf{b}$ in the generators of $\mathcal{H}$.
For origin choice 2, fractions $\frac{1}{4}$ and $\frac{3}{4}$ appear in all 'coordinates' of the generator (3) $\bar{y}+\frac{1}{4}, x+\frac{3}{4}, z+\frac{1}{4}$ of $\mathcal{G}$. As a consequence, translational parts with vectors $(\frac{p}{4}+\frac{1}{4})\mathbf{a}$ and $(\frac{3p}{4}-\frac{5}{4})\mathbf{b}$ appear if $p \equiv 3 \pmod 4$. On the other hand, translational parts with vectors $(\frac{p}{4}-\frac{1}{4})\mathbf{a}$, $(\frac{3p}{4}-\frac{3}{4})\mathbf{b}$ are introduced in the generators of $\mathcal{H}$ if $p \equiv 1 \pmod 4$ holds.
Another consequence of the fractions $\frac{1}{4}$ and $\frac{3}{4}$ occurring in the generator (3) of $\mathcal{G}$ is the difference in the origin shifts. They are $\frac{1}{2}+u$, v, 0 for $p \equiv 3 \pmod 4$ and u, v, 0 for $p \equiv 1 \pmod 4$. Thus, the one series in origin choice 1 for odd p is split into two series in origin choice 2 for $p \equiv 3 \pmod 4$ and $p \equiv 1 \pmod 4$.[3]

2.1.6. Minimal supergroups

2.1.6.1. *General description*

In the previous sections, the relation $\mathcal{H} < \mathcal{G}$ was seen from the viewpoint of the group $\mathcal{G}$. In this case, $\mathcal{H}$ was a subgroup of $\mathcal{G}$. However, the same relation may be viewed from the group $\mathcal{H}$. In this case, $\mathcal{G} > \mathcal{H}$ is a *supergroup* of $\mathcal{H}$. As for the subgroups of $\mathcal{G}$, *cf.* Section 1.2.6, different kinds of supergroups of $\mathcal{H}$ may be distinguished. The following definitions are obvious.

Definition 2.1.6.1.1. Let $\mathcal{H} < \mathcal{G}$ be a maximal subgroup of $\mathcal{G}$. Then $\mathcal{G} > \mathcal{H}$ is called a *minimal supergroup* of $\mathcal{H}$. If $\mathcal{H}$ is a *translationengleiche* subgroup of $\mathcal{G}$ then $\mathcal{G}$ is a *translationengleiche supergroup* (*t-supergroup*) of $\mathcal{H}$. If $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a *klassengleiche supergroup* (*k-supergroup*) of $\mathcal{H}$. If $\mathcal{H}$ is an isomorphic subgroup of $\mathcal{G}$, then $\mathcal{G}$ is an *isomorphic supergroup* of $\mathcal{H}$. If $\mathcal{H}$ is a general subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a *general supergroup* of $\mathcal{H}$. □

The search for supergroups of space groups is much more difficult than the search for subgroups. One of the reasons for this difficulty is that the search for subgroups $\mathcal{H} < \mathcal{G}$ is restricted to the elements of the space group $\mathcal{G}$ itself, whereas the search for supergroups $\mathcal{G} > \mathcal{H}$ has to take into account the whole (continuous) group $\mathcal{E}$ of all isometries. For example, there are only a finite number of subgroups $\mathcal{H}$ of any space group $\mathcal{G}$ for any given index i. On the other hand, there may not only be an infinite number of supergroups $\mathcal{G}$ of a space group $\mathcal{H}$ for a finite index i but even an uncountably infinite number of supergroups of $\mathcal{H}$.

Example 2.1.6.1.2.
Let $\mathcal{H} = P1$. Then there is an infinite number of t-supergroups $P\bar{1}$ of index 2 because there is no restriction for the sites of the centres of inversion and thus of the conventional origin of $P\bar{1}$.

In the tables of this volume, a supergroup $\mathcal{G}$ of a space group $\mathcal{H}$ is listed by its type if $\mathcal{H}$ is listed as a subgroup of $\mathcal{G}$. The entry contains at least the index of $\mathcal{H}$ in $\mathcal{G}$, the conventional HM symbol of $\mathcal{G}$ and its space-group number. Additional data may be given for *klassengleiche* supergroups. More details, *e.g.* the representatives of the general position or the generators as well as the transformation matrix and the origin shift, would only duplicate the subgroup data. The number of supergroups belonging to one entry can neither be concluded from the subgroup data nor is it listed among the supergroup data.

Like the subgroup data, the supergroup data are also partitioned into blocks.

2.1.6.2. *I Minimal translationengleiche supergroups*

For each space group $\mathcal{H}$, under this heading are listed those space-group types $\mathcal{G}$ for which $\mathcal{H}$ appears as an entry under the heading **I Maximal *translationengleiche* subgroups**. The listing consists of the index in brackets [...], the conventional HM symbol and (in parentheses) the space-group number (...). The space groups are ordered by ascending space-group number. If this line is empty, the heading is printed nevertheless and the content is announced by 'none', as in $P6/mmm$, No. 191.

The supergroups listed on the line **I Minimal *translationengleiche* supergroups** are realized only if the lattice conditions of $\mathcal{H}$ fulfil the lattice conditions for $\mathcal{G}$. For example, if $\mathcal{G} = P422$, No. 89, is a supergroup of $\mathcal{H} = P222$, No. 16, two of the three independent lattice parameters a, b, c of $P222$ must be equal (or in crystallographic practice, approximately equal). These must be a and b if c is the tetragonal axis, b and c if a is the tetragonal axis or c and a if b is the tetragonal axis. In the latter two cases, the setting of $P222$ has to be adapted to the conventional c-axis setting of $P422$. For the cubic supergroup $P23$, No. 195, all three lattice parameters of $P222$ must be (approximately) equal. Such conditions are always to be taken into consideration if the t-supergroup belongs to a different crystal family[4] to the original group. Therefore, for $\mathcal{H} = P222$ there is no lattice condition for the supergroup $\mathcal{G} = Pmmm$ because $P222$ and $Pmmm$ belong to the same crystal family.

2.1.6.3. *II Minimal non-isomorphic klassengleiche supergroups*

Klassengleiche supergroups $\mathcal{G} > \mathcal{H}$ always belong to the crystal family of $\mathcal{H}$. Therefore, there are no restrictions for the lattice parameters of $\mathcal{H}$.

The block **II Minimal non-isomorphic *klassengleiche* supergroups** is divided into two subblocks with the headings **Additional centring translations** and **Decreased unit cell**. If both subblocks are empty, only the heading of the block is listed, stating 'none' for the content of the block, as in $P6/mmm$, No. 191.

If at least one of the subblocks is non-empty, then the heading of the block and the headings of both subblocks are listed. An

[3] F. Gähler (private communication) has shown that such a splitting can be avoided if one allows the prime p to enter the formulae for the origin shifts. In these tables we have not made use of this possibility in order to keep the origin shifts in the same form for all space groups $\mathcal{G}$.

[4] For the term 'crystal family' *cf.* Section 1.2.5.2, or, for more details, *IT* A, Section 8.2.7.

empty subblock is then designated by 'none'; in the other subblock the supergroups are listed. The kind of listing depends on the subblock. Examples may be found in the tables of *P*222, No. 16, and $Fd\bar{3}c$, No. 228.

Under the heading 'Additional centring translations', the supergroups are listed by their indices and either by their nonconventional HM symbols, with the space-group numbers and the standard HM symbols in parentheses, or by their conventional HM symbols and only their space-group numbers in parentheses. Examples are provided by space group *Pbca*, No. 61, with both subblocks non-empty and by space group *P*222, No. 16, with supergroups only under the heading 'Additional centring translations'.

Under the heading 'Decreased unit cell' each supergroup is listed by its index and by its lattice relations, where the basis vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{c}'$ refer to the supergroup $\mathcal{G}$ and the basis vectors **a**, **b** and **c** to the original group $\mathcal{H}$. After these data are listed either the nonconventional HM symbol, followed by the space-group number and the conventional HM symbol in parentheses, or the conventional HM symbol with the space-group number in parentheses. Examples are provided again by space group *Pbca*, No. 61, with both subblocks occupied and space group $F\bar{4}3m$, No. 216, with an empty subblock 'Additional centring translations' but data under the heading 'Decreased unit cell'.

2.1.6.4. *Isomorphic supergroups*

Each space group $\mathcal{G}$ has an infinite number of isomorphic subgroups $\mathcal{H}$ because the number of primes is infinite. For the same reason, each space group $\mathcal{H}$ has an infinite number of isomorphic supergroups $\mathcal{G}$. They are not listed in the tables of this volume because they are implicitly listed among the subgroup data.

2.1.7. The subgroup graphs

2.1.7.1. *General remarks*

The group–subgroup relations between the space groups may also be described by graphs. This way is chosen in Chapters 2.4 and 2.5. Graphs for the group–subgroup relations between crystallographic point groups have been published, for example, in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and in *IT* A (2002), Fig. 10.1.4.3. Three kinds of graphs for subgroups of space groups have been constructed and can be found in the literature:

(1) Graphs for *t*-subgroups, such as the graphs of Ascher (1968).
(2) Graphs for *k*-subgroups, such as the graphs for cubic space groups of Neubüser & Wondratschek (1966).
(3) Mixed graphs, combining *t*- and *k*-subgroups. These are used, for example, when relations between existing or suspected crystal structures are to be displayed. An example is the 'family tree' of Bärnighausen (1980), Fig. 15, now called a *Bärnighausen tree*.

A complete collection of graphs of the first two kinds is presented in this volume: in Chapter 2.4 those displaying the *translationengleiche* or *t*-subgroup relations and in Chapter 2.5 those for the *klassengleiche* or *k*-subgroup relations. Neither type of graph is restricted to maximal subgroups but both contain *t*- or *k*-subgroups of higher indices, with the exception of isomorphic subgroups, *cf.* Section 2.1.7.3 below.

The group–subgroup relations are direct relations between the space groups themselves, not between their types. However, each such relation is valid for a pair of space groups, one from each of the types, and for each space group of a given type there exists a corresponding relation. In this sense, one can speak of a relation between the space-group types, keeping in mind the difference between space groups and space-group types, *cf.* Section 1.2.5.3.

The space groups in the graphs are denoted by the standard HM symbols and the space-group numbers. In each graph, each space-group type is displayed at most once. Such graphs are called *contracted graphs* here. Without this contraction, the more complex graphs would be much too large for the page size of this volume.

The symbol of a space group $\mathcal{G}$ is connected by uninterrupted straight lines with the symbols of all maximal non-isomorphic subgroups $\mathcal{H}$ or minimal non-isomorphic supergroups $\mathcal{S}$ of $\mathcal{G}$. In general, the *maximal subgroups* of $\mathcal{G}$ are drawn on a *lower level* than $\mathcal{G}$; in the same way, the *minimal supergroups* of $\mathcal{G}$ are mostly drawn on a *higher level* than $\mathcal{G}$. For exceptions see Section 2.1.7.3. Multiple lines may occur in the graphs for *t*-subgroups. They are explained in Section 2.1.7.2. No indices are attached to the lines. They can be taken from the corresponding subgroup tables of Chapter 2.3, and are also provided by the general formulae of Section 1.2.8. For the *k*-subgroup graphs, they are further specified at the end of Section 2.1.7.3.

2.1.7.2. *Graphs for translationengleiche subgroups*

Let $\mathcal{G}$ be a space group and $\mathcal{T}(\mathcal{G})$ the normal subgroup of all its translations. Owing to the isomorphism between the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ and the point group $\mathcal{P}_{\mathcal{G}}$, see Section 1.2.5.4, according to the first isomorphism theorem, Ledermann (1976), *t*-subgroup graphs are the same (up to the symbols) as the corresponding graphs between point groups. However, in this volume, the graphs are not complete but are contracted by displaying each space-group type at most once. This contraction may cause the graphs to look different from the point-group graphs and also different for different space groups of the same point group, *cf.* Example 2.1.7.2.1.

One can indicate the connections between a space group $\mathcal{G}$ and its maximal subgroups in different ways. In the contracted *t*-subgroup graphs one line is drawn for each conjugacy class of maximal subgroups of $\mathcal{G}$. Thus, a line represents the connection to an individual subgroup only if this is a normal maximal subgroup of $\mathcal{G}$, otherwise it represents the connection to more than one subgroup. The conjugacy relations are not necessarily transferable to non-maximal subgroups, *cf.* Example 2.1.7.2.2. On the other hand, multiple lines are possible, see the examples. Although it is not in general possible to reconstruct the complete graph from the contracted one, the content of information of such a graph is higher than that of a graph which is drawn with simple lines only.

The graph for the space group at its top also contains the contracted graphs for all subgroups which occur in it, see the remark below Example 2.1.7.2.2.

Owing to lack of space for the large graphs, in all graphs of *t*-subgroups the group *P*1, No. 1, and its connections have been omitted. Therefore, to obtain the full graph one has to supplement the graphs by *P*1 at the bottom and to connect *P*1 by one line to each of the symbols that have no connection downwards.

Within the same graph, symbols on the same level indicate subgroups of the same index relative to the group at the top. The distance between the levels indicates the size of the index. For a more detailed discussion, see Example 2.1.7.2.2. For the sequence and the numbers of the graphs, see the paragraph below Example 2.1.7.2.2.

Example 2.1.7.2.1.

Compare the *t*-subgroup graphs in Figs. 2.4.4.2, 2.4.4.3 and 2.4.4.8 of *Pnna*, No. 52, *Pmna*, No. 53, and *Cmce*, No. 64, respectively. The *complete* (uncontracted) *graphs* would have the shape of the graph of the point group *mmm* with *mmm* at the top (first level), seven point groups[5] (222, *mm*2, *m*2*m*, 2*mm*, $112/m$, $12/m1$ and $2/m11$) in the second level, seven point groups (112, 121, 211, 11*m*, 1*m*1, *m*11 and $\bar{1}$) in the third level and the point group 1 at the bottom (fourth level). The group *mmm* is connected to each of the seven subgroups at the second level by one line. Each of the groups of the second level is connected with three groups of the third level by one line. All seven groups of the third level are connected by one line each with the point group 1 at the bottom.

The *contracted graph* of the point group *mmm* would have *mmm* at the top, three point-group types (222, *mm*2 and $2/m$) at the second level and three point-group types (2, *m* and $\bar{1}$) at the third level. The point group 1 at the bottom would not be displayed (no fourth level). Single lines would connect *mmm* with 222, *mm*2 with 2, $2/m$ with 2, $2/m$ with *m* and $2/m$ with $\bar{1}$; a double line would connect *mm*2 with *m*; triple lines would connect *mmm* with *mm*2, *mmm* with $2/m$ and 222 with 2.

The number of fields in a contracted *t*-subgroup graph is between the numbers of fields in the full and in the contracted point-group graphs. The graph in Fig. 2.4.4.2 of *Pnna*, No. 52, has six space-group types at the second level and four space-group types at the third level. For the graph in Fig. 2.4.4.3 of *Pmna*, No. 53, these numbers are seven and five and for the graph in Fig. 2.4.4.8 of *Cmce*, No. 64 (formerly *Cmca*), the numbers are seven and six. However, in all these graphs the number of connections is always seven from top to the second level and three from each field of the second level downwards to the ground level, independent of the amount of contraction and of the local multiplicity of lines.

Example 2.1.7.2.2.

Compare the *t*-subgroup graphs shown in Fig. 2.4.1.1 for $Pm\bar{3}m$, No. 221, and Fig. 2.4.1.5, $Fm\bar{3}m$, No. 225. These graphs are contracted from the point-group graph $m\bar{3}m$. There are altogether nine levels (without the lowest level of *P*1). The indices relative to the top space groups $Pm\bar{3}m$ and $Fm\bar{3}m$ are 1, 2, 3, 4, 6, 8, 12, 16 and 24, corresponding to the point-group orders 48, 24, 16, 12, 8, 6, 4, 3 and 2, respectively. The height of the levels in the graphs reflects the index; the distances between the levels are slightly distorted in order to adapt to the density of the lines. From the top space-group symbol there are five lines to the symbols of maximal subgroups: The three symbols at the level of index 2 are those of cubic normal subgroups, the one (tetragonal) symbol at the level of index 3 represents a conjugacy class of three, the symbol $R\bar{3}m$, No. 166, at the level of index 4 represents a conjugacy class of four subgroups.

The graphs differ in the levels of the indices 12 and 24 (orthorhombic, monoclinic and triclinic subgroups) by the number of symbols (nine and seven for index 12, five and three for index 24). The number of lines between neighbouring connected levels depends only on the number and kind of symbols in the upper level. This property makes such graphs particularly useful.

However, for non-maximal subgroups the conjugacy relations may not hold. For example, in Fig. 2.4.1.1, the space group *P*222 has three normal maximal subgroups of type *P*2 and is thus connected to its symbol by a triple line, although these subgroups are conjugate subgroups of the non-minimal supergroup $Pm\bar{3}m$.

The *t*-subgroup graphs in Figs. 2.4.1.1 and 2.4.1.5 contain the *t*-subgroups of $Pm\bar{3}m$ (221) and $Fm\bar{3}m$ (225) and their relations. In addition, the *t*-subgroup graph of $Pm\bar{3}m$ includes the *t*-subgroup graphs of *P*432, $P\bar{4}3m$, $Pm\bar{3}$, *P*23, $P4/mmm$, $P\bar{4}2m$, $P\bar{4}m2$, *P*4*mm*, $R\bar{3}m$, *R*3*m etc.*, that of $Fm\bar{3}m$ includes those of *F*432, $F\bar{4}3m$, $Fm\bar{3}$, $I4/mmm$, also $R\bar{3}m$ *etc*. Thus, many other graphs can be extracted from the two basic graphs. The same holds for the other graphs displayed in Figs. 2.4.1.2 to 2.4.4.8: each of them includes the contracted graphs of all its subgroups. For this reason one does not need 229 or 218 different graphs to cover all *t*-subgroup graphs of the 229 space-group types but only 37 (*P*1 can be excluded as trivial).

The preceding Example 2.1.7.2.2 suggests that one should choose the graphs in such a way that their number can be kept small. It is natural to display the 'big' graphs first and later those smaller graphs that are still missing. This procedure is behind the sequence of the *t*-subgroup graphs in this volume.

(1) The ten graphs of $Pm\bar{3}m$, No. 221, to $Ia\bar{3}d$, No. 230, form the first set of graphs in Figs. 2.4.1.1 to 2.4.1.10.
(2) There are a few cubic space groups left which do not appear in the first set. They are covered by the graphs of $P4_132$ (213), $P4_332$ (212) and $Pa\bar{3}$ (205). These graphs have large parts in common so that they can be united in Fig. 2.4.1.11.
(3) No cubic space group is left now, but only eight tetragonal space groups of crystal class $4/mmm$ have appeared up to now. Among them are all graphs for $4/mmm$ space groups with an *I* lattice which are contained in Figs. 2.4.1.5 to 2.4.1.8 of the *F*-centred cubic space groups. The next 12 graphs, Figs. 2.4.2.1 to 2.4.2.12, are those for the space groups of the crystal class $4/mmm$ with lattice symbol *P* and different third and fourth constituents of the HM symbol. They start with $P4/mcc$, No. 124, and end with $P4_2/ncm$, No. 138.
(4) Two (enantiomorphic) tetragonal space-group types are left which are compiled in Fig. 2.4.2.13.
(5) The next set is formed by the four graphs in Figs. 2.4.3.1 to 2.4.3.4 of the hexagonal space groups $P6/mmm$, No. 191, to $P6_3/mmc$, No. 194. The hexagonal and trigonal enantiomorphic space groups do not appear in these graphs. They are combined in Fig. 2.4.3.5, the last one of hexagonal origin.
(6) Several orthorhombic space groups are still left. They are treated in the eight graphs in Figs. 2.4.4.1 to 2.4.4.8, from *Pmma*, No. 51, to *Cmce*, No. 64 (formerly *Cmca*).
(7) For each space group, the contracted graph of all its *t*-subgroups is provided in at least one of these 37 graphs.

For the index of a maximal *t*-subgroup, Lemma 1.2.8.2.3 is repeated: the index of a maximal non-isomorphic subgroup $\mathcal{H}$ is always 2 for oblique, rectangular and square plane groups and for triclinic, monoclinic, orthorhombic and tetragonal space groups $\mathcal{G}$. The index is 2 or 3 for hexagonal plane groups and for trigonal and hexagonal space groups $\mathcal{G}$. The index is 2, 3 or 4 for cubic space groups $\mathcal{G}$.

2.1.7.3. *Graphs for klassengleiche subgroups*

There are 29 graphs for *klassengleiche* or *k*-subgroups, one for each crystal class with the exception of the crystal classes 1, $\bar{1}$ and $\bar{6}$ with only one space-group type each: *P*1, No. 1, $P\bar{1}$, No. 2, and $P\bar{6}$, No. 174, respectively. The sequence of the graphs is

[5] The HM symbols used here are nonconventional. They display the setting of the point group and follow the rules of *IT* A, Section 2.2.4.

determined by the sequence of the point groups in *IT* A, Table 2.1.2.1, fourth column. The graphs of $\overline{4}$, $\overline{3}$ and $6/m$ are nearly trivial, because to these crystal classes only two space-group types belong. The graphs of $mm2$ with 22, of mmm with 28 and of $4/mmm$ with 20 space-group types are the most complicated ones.

Isomorphic subgroups are special cases of *k*-subgroups. With the exception of both partners of the enantiomorphic space-group types, isomorphic subgroups are not displayed in the graphs. The explicit display of the isomorphic subgroups would add an infinite number of lines from each field for a space group back to this field, or at least one line (*e.g.* a circle) implicitly representing the infinite number of isomorphic subgroups, see the tables of maximal subgroups of Chapter 2.3.[6] Such a line would have to be attached to every space-group symbol. Thus, there would be no more information.

Nevertheless, connections between isomorphic space groups are included indirectly if the group–subgroup chain encloses a space group of another type. In this case, a space group $\mathcal{X}$ may be a subgroup of a space group $\mathcal{Y}$ and $\mathcal{Y}'$ a subgroup of $\mathcal{X}$, where $\mathcal{Y}$ and $\mathcal{Y}'$ belong to the same space-group type. The subgroup chain is then $\mathcal{Y} - \mathcal{X} - \mathcal{Y}'$. The two space groups $\mathcal{Y}$ and $\mathcal{Y}'$ are not identical but isomorphic. Whereas in general the label for the subgroup is positioned at a lower level than that for the original space group, for such relations the symbols for $\mathcal{X}$ and $\mathcal{Y}$ can only be drawn on the same level, connected by horizontal lines. If this happens at the top of a graph, the top level is occupied by more than one symbol (the number of symbols in the top level is the same as the number of symmorphic space-group types of the crystal class).

Horizontal lines are drawn as left or right arrows depending on the kind of relation. The arrow is always directed from the supergroup to the subgroup. If the relation is two-sided, as is always the case for enantiomorphic space-group types, then the relation is displayed by a pair of horizontal lines, one of them formed by a right and the other by a left arrow. In the graph in Fig. 2.5.1.5 for crystal class $mm2$, the connections of $Pmm2$ with $Cmm2$ and with $Amm2$ are displayed by double-headed arrows instead. Furthermore, some arrows in Fig. 2.5.1.5, crystal class $mm2$, and Fig. 2.5.1.6, mmm, are dashed or dotted in order to better distinguish the different lines and to increase clarity.

The different kinds of relations are demonstrated in the following examples.

Example 2.1.7.3.1.

In the graph in Fig. 2.5.1.1, crystal class 2, a space group $P2$ may be a subgroup of index 2 of a space group $C2$ by 'Loss of centring translations'. On the other hand, subgroups of $P2$ in the block 'Enlarged unit cell', $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $C2$ (3) belong to the type $C2$, see the tables of maximal subgroups in Chapter 2.3. Therefore, both symbols are drawn at the same level and are connected by a pair of arrows pointing in opposite directions. Thus, the top level is occupied twice. In the graph in Fig. 2.5.1.2 of crystal class m, both the top level and the bottom level are occupied twice.

Example 2.1.7.3.2.

There are four symbols at the top level of the graph in Fig. 2.5.1.4, crystal class 222. Their relations are rather complicated. Whereas one can go (by index 2) from $P222$ directly to a subgroup of type $C222$ and *vice versa*, the connection from $F222$ directly to $C222$ is one-way. One always has to pass $C222$ on the way from $F222$ to a subgroup of the types $P222$ or $I222$. Thus, the only maximal subgroup of $F222$ among these groups is $C222$. One can go directly from $P222$ to $F222$ but not to $I222$ *etc*.

Because of the horizontal connecting arrows, it is clear that there cannot be much correspondence between the level in the graphs and the subgroup index. However, in no graph is a subgroup positioned at a higher level than the supergroup.

Example 2.1.7.3.3.

Consider the graph in Fig. 2.5.1.6 for crystal class mmm. To the space group $Cmmm$ (65) belong maximal non-isomorphic subgroups of the 11 space-group types (from left to right) $Ibam$ (72), $Cmcm$ (63), $Imma$ (74), $Pmmn$ (59), $Pbam$ (55), $Pban$ (50), $Pmma$ (51), $Pmna$ (53), $Cccm$ (66), $Pmmm$ (47) and $Immm$ (71). Although all of them have index 2, their symbols are positioned at very different levels of the graph.

The table for the subgroups of $Cmmm$ in Chapter 2.3 lists 22 non-isomorphic *k*-subgroups of index 2, because some of the space-group types mentioned above are represented by two or four different subgroups. This multiplicity cannot be displayed by multiple lines because the density of the lines in some of the *k*-subgroup graphs does not permit this kind of presentation, *e.g.* for mmm. The multiplicity may be taken from the subgroup tables in Chapter 2.3, where each non-isomorphic subgroup is listed individually.

Consider the connections from $Cmmm$ (65) to $Pbam$ (55). There are among others: the direct connection of index 2, the connection of index 4 over $Ibam$ (72), the connection of index 8 over $Imma$ (74) and $Pmma$ (51). Thus, starting from the same space group of type $Cmmm$ one arrives at different space groups of the type $Pbam$ with different unit cells but all belonging to the same space-group type and thus represented by the same field of the graph.

The index of a *k*-subgroup is restricted by Lemma 1.2.8.2.3 and by additional conditions. For the following statements one has to note that enantiomorphic space groups are isomorphic.

(1) A non-isomorphic maximal *k*-subgroup of an oblique, rectangular or tetragonal plane group or of a triclinic, monoclinic, orthorhombic or tetragonal space group always has index 2.
(2) In general, a non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a trigonal space group $\mathcal{G}$ has index 3. Exceptions are the pairs $P3m1$–$P3c1$, $P31m$–$P31c$, $R3m$–$R3c$, $P\overline{3}1m$–$P\overline{3}1c$, $P\overline{3}m1$–$P\overline{3}c1$ and $R\overline{3}m$–$R\overline{3}c$ with space-group Nos. between 156 and 167. They have index 2.
(3) A non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a hexagonal space group has index 2 or 3.
(4) A non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a cubic space group $\mathcal{G}$ has either index 2 or index 4. The index is 2 if $\mathcal{G}$ has an I lattice and $\mathcal{H}$ a P lattice or if $\mathcal{G}$ has a P lattice and $\mathcal{H}$ an F lattice. The index is 4 if $\mathcal{G}$ has an F lattice and $\mathcal{H}$ a P lattice or if $\mathcal{G}$ has a P lattice and $\mathcal{H}$ an I lattice.

2.1.7.4. *Graphs for plane groups*

There are no graphs for plane groups in this volume. The four graphs for *t*-subgroups of plane groups are apart from the symbols the same as those for the corresponding space groups: $p4mm$–$P4mm$, $p6mm$–$P6mm$, $p2mg$–$Pma2$ and $p2gg$–$Pba2$, where the graphs for the space groups are included in the *t*-subgroup graphs in Figs. 2.4.1.1, 2.4.3.1, 2.4.2.1 and 2.4.2.3, respectively.

[6] One could contemplate adding one line for each series of maximal isomorphic subgroups. However, the number of series depends on the rules that define the distribution of the isomorphic subgroups into the series and is thus not constant.

The *k*-subgroup graphs are trivial for the plane groups *p*1, *p*2, *p*4, *p*3, *p*6 and *p*6*mm* because there is only one plane group in its crystal class. The graphs for the crystal classes 4*mm* and 3*m* consist of two plane groups each: *p*4*mm* and *p*4*gm*, *p*3*m*1 and *p*31*m*. Nevertheless, the graphs are different: the relation is one-sided for the tetragonal plane-group pair as it is in the space-group pair $P6/m$ (175)–$P6_3/m$ (176) and it is two-sided for the hexagonal plane-group pair as it is in the space-group pair $P\overline{4}$ (81)–$I\overline{4}$ (82). The graph for the three plane groups of the crystal class *m* corresponds to the space-group graph for the crystal class 2.

Finally, the graph for the four plane groups of crystal class 2*mm* has no direct analogue among the *k*-subgroup graphs of the space groups. It can be obtained, however, from the graph in Fig. 2.5.1.3 of crystal class $2/m$ by removing the fields of $C2/c$ (15) and $P2_1/m$ (11) with all their connections to the remaining fields. The replacements are then: $C2/m$ (12) by *c*2*mm* (9), $P2/m$ (10) by *p*2*mm* (6), $P2/c$ (13) by *p*2*mg* (7) and $P2_1/c$ (14) by *p*2*gg* (8).

2.1.7.5. *Application of the graphs*

If a subgroup is not maximal then there must be a group–subgroup chain $\mathcal{G}$–$\mathcal{H}$ of maximal subgroups with more than two members which connects $\mathcal{G}$ with $\mathcal{H}$. There are three possibilities: $\mathcal{H}$ may be a *t*-subgroup or a *k*-subgroup or a general subgroup of $\mathcal{G}$. In the first two cases, the application of the graphs is straightforward because at least one of the graphs will permit one to find the possible chains directly. If $\mathcal{H}$ is a *k*-subgroup of $\mathcal{G}$, isomorphic subgroups have to be included if necessary. If $\mathcal{H}$ is a general subgroup of $\mathcal{G}$ one has to combine *t*- and *k*-subgroup graphs, but the problem is only slightly more complicated. This is because for a general subgroup $\mathcal{H} < \mathcal{G}$, Hermann's theorem 1.2.8.1.2 states the existence of an intermediate group $\mathcal{M}$ with $\mathcal{H} < \mathcal{M} < \mathcal{G}$ and the properties $\mathcal{H} < \mathcal{M}$ is a *k*-subgroup of $\mathcal{M}$ and $\mathcal{M} < \mathcal{G}$ is a *t*-subgroup of $\mathcal{G}$.

Thus, however long and complicated the real chain may be, there is also always a chain for which only two graphs are needed: a *t*-subgroup graph for the relation between $\mathcal{G}$ and $\mathcal{M}$ and a *k*-subgroup graph for the relation between $\mathcal{M}$ and $\mathcal{H}$.

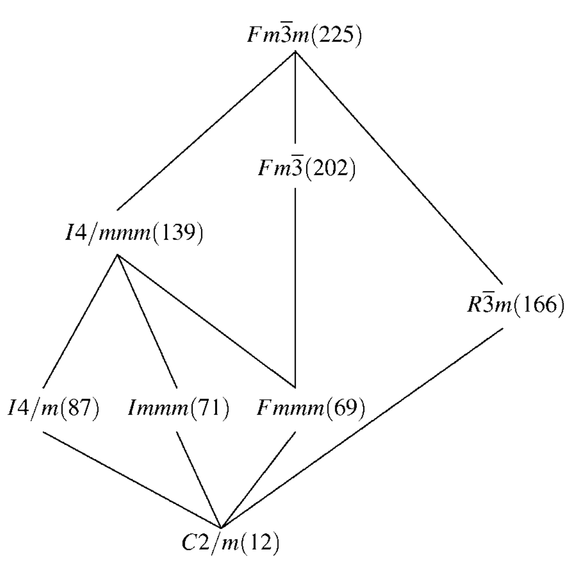

Fig. 2.1.7.1. Contracted graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to those subgroups with index 12 which belong to the space-group type $C2/m$ (12). The graph forms part of the total contracted graph of *t*-subgroups of $Fm\overline{3}m$ (Fig. 2.4.1.5).

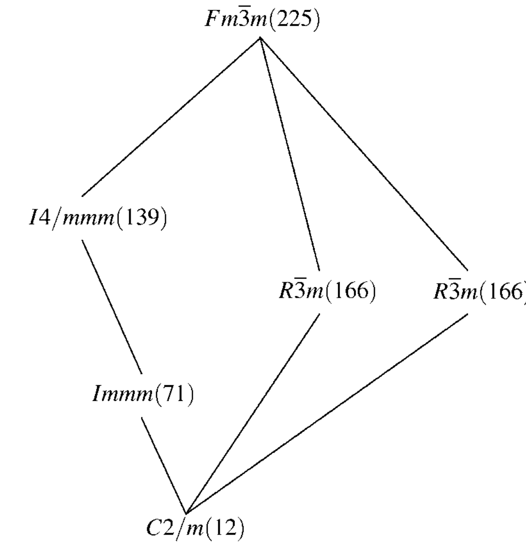

Fig. 2.1.7.2. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one representative of those six $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the $\langle 110 \rangle$ directions of $Fm\overline{3}m$.

There is, however, a severe shortcoming to using contracted graphs for the analysis of group–subgroup relations, and great care has to be taken in such investigations. All subgroups $\mathcal{H}_j$ with the same space-group type are represented by the same field of the graph, but these different non-maximal subgroups may permit different routes to a common original (super)group.

Example 2.1.7.5.1.

An example for *translationengleiche* subgroups is provided by the group–subgroup chain $Fm\overline{3}m$ (225)–$C2/m$ (12) of index 12. The contracted graph may be drawn by the program *Subgroupgraph* from the Bilbao Crystallographic Server, http://www.cryst.ehu.es/. It is shown in Fig. 2.1.7.1; each field represents all occurring subgroups of a space-group type: $I4/mmm$ (139) represents three subgroups, $R\overline{3}m$ (166) represents four subgroups, ... and $C2/m$ (12) represents nine subgroups belonging to two conjugacy classes. Fig. 2.1.7.1 is part of the contracted total graph of the *translationengleiche* subgroups of the space group $Fm\overline{3}m$, which is displayed in Fig.

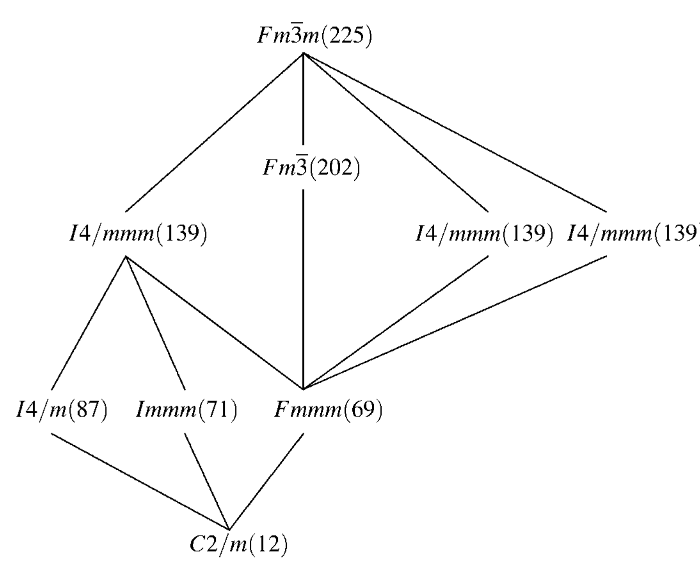

Fig. 2.1.7.3. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one representative of those three $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the $\langle 001 \rangle$ directions of $Fm\overline{3}m$.

2.4.1.5. With *Subgroupgraph* one can also obtain the *complete graph* between $Fm\overline{3}m$ and the set of all nine subgroups of the type $C2/m$. It is too large to be reproduced here.

More instructive are the complete graphs for different single subgroups of the type $C2/m$ of $Fm\overline{3}m$. They can be obtained with the program *Symmodes* from the same server as above. In Fig. 2.1.7.2 such a graph is displayed for one of the six subgroups of type $C2/m$ of index 12 whose monoclinic axes point in the $\langle 110 \rangle$ directions of $Fm\overline{3}m$. Similarly, in Fig. 2.1.7.3 the complete graph is drawn for one of the three subgroups of $C2/m$ of index 12 whose monoclinic axes point in the $\langle 001 \rangle$ directions of $Fm\overline{3}m$. It differs markedly from the contracted graph and from the first complete graph. It is easily seen that it may be very misleading to use the contracted graph or the wrong individual complete graph instead of the right individual complete graph.

The following example deals with general subgroups.

Example 2.1.7.5.2.

The crystal structures of $SrTiO_3$ and $KCuF_3$ both belong to the space-group type $I4/mcm$, No. 140. They can be derived by different distortions from the same ideal perovskite ABX_3 structure with the space group $Pm\overline{3}m$, No. 221. Common to both chains is Hermann's group $\mathcal{M}$ of space group $P4/mmm$, No. 123, and the unit cell of ABX_3. This is the only intermediate group for $SrTiO_3$. For the pair ABX_3–$KCuF_3$, on the other hand, there exists another chain with an intermediate space group of type $Fm\overline{3}c$, No. 226. The combination of the graph in Fig. 2.4.1.1 for *t*-subgroups with the graph in Fig. 2.5.2.7 for *k*-subgroups is thus possible for both crystal–chemical relations. The combination of the graph in Fig. 2.5.5.5 for *k*-subgroups with the graph in Fig. 2.4.1.6 for *t*-subgroups is, however, only meaningful for the chain ABX_3–$KCuF_3$. This cannot be concluded from the contracted graphs but can be seen from the complete graph, as displayed in Fig. 1 of Wondratschek & Aroyo (2001).

references

$p1$ No. 1 $p1$

Generators selected (1); $t(1,0)$; $t(0,1)$

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
1	*a*	1	(1) x, y

I Maximal *translationengleiche* subgroups none

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$

$p1$ (1)	$\langle 1 \rangle$	$2\mathbf{a}, \mathbf{b}$

[2] $\mathbf{b}' = 2\mathbf{b}$

$p1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, 2\mathbf{b}$

[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$

$c1$ (1, $p1$)	$\langle 1 \rangle$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}$

[3] $\mathbf{a}' = 3\mathbf{a}$

$p1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, \mathbf{b}$

[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -\mathbf{a}+\mathbf{b}$

$p1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}$

[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -2\mathbf{a}+\mathbf{b}$

$p1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}$

[3] $\mathbf{b}' = 3\mathbf{b}$

$p1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, 3\mathbf{b}$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = -q\mathbf{a}+\mathbf{b}$

$p1$ (1)	$\langle 1 \rangle$ $p > 1$; $0 \le q < p$ no conjugate subgroups	$p\mathbf{a}, -q\mathbf{a}+\mathbf{b}$

[p] $\mathbf{b}' = p\mathbf{b}$

$p1$ (1)	$\langle 1 \rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, p\mathbf{b}$

I Minimal *translationengleiche* supergroups

[2] $p2$ (2); [2] pm (3); [2] pg (4); [2] cm (5); [3] $p3$ (13)

II Minimal non-isomorphic *klassengleiche* supergroups none

$p2$ No. 2 $p2$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	*e*	1	(1) x, y (2) $\bar{x}, \bar{y}$

I Maximal *translationengleiche* subgroups

[2] $p1$ (1)	1		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$			
$p2$ (2)	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{b}$	
$p2$ (2)	$\langle 2 + (1,0) \rangle$	$2\mathbf{a}, \mathbf{b}$	$1/2, 0$
[2] $\mathbf{b}' = 2\mathbf{b}$			
$p2$ (2)	$\langle 2 \rangle$	$\mathbf{a}, 2\mathbf{b}$	
$p2$ (2)	$\langle 2 + (0,1) \rangle$	$\mathbf{a}, 2\mathbf{b}$	$0, 1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
$c2$ (2, $p2$)	$\langle 2 \rangle$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}$	
$c2$ (2, $p2$)	$\langle 2 + (1,0) \rangle$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}$	$1/2, 0$
[3] $\mathbf{a}' = 3\mathbf{a}$			
$\{$ $p2$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{b}$	
$p2$ (2)	$\langle 2 + (2,0) \rangle$	$3\mathbf{a}, \mathbf{b}$	$1, 0$
$p2$ (2)	$\langle 2 + (4,0) \rangle$	$3\mathbf{a}, \mathbf{b}$	$2, 0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -\mathbf{a}+\mathbf{b}$			
$\{$ $p2$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}$	
$p2$ (2)	$\langle 2 + (2,0) \rangle$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}$	$1, 0$
$p2$ (2)	$\langle 2 + (4,0) \rangle$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}$	$2, 0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -2\mathbf{a}+\mathbf{b}$			
$\{$ $p2$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}$	
$p2$ (2)	$\langle 2 + (2,0) \rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}$	$1, 0$
$p2$ (2)	$\langle 2 + (4,0) \rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}$	$2, 0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
$\{$ $p2$ (2)	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}$	
$p2$ (2)	$\langle 2 + (0,2) \rangle$	$\mathbf{a}, 3\mathbf{b}$	$0, 1$
$p2$ (2)	$\langle 2 + (0,4) \rangle$	$\mathbf{a}, 3\mathbf{b}$	$0, 2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = -q\mathbf{a}+\mathbf{b}$			
$p2$ (2)	$\langle 2 + (2u,0) \rangle$ $p > 2$; $0 \le q < p$; $0 \le u < p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a}, -q\mathbf{a}+\mathbf{b}$	$u, 0$
[p] $\mathbf{b}' = p\mathbf{b}$			
$p2$ (2)	$\langle 2 + (0,2u) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}$	$0, u$

I Minimal *translationengleiche* supergroups

[2] *p*2*mm* (6); [2] *p*2*mg* (7); [2] *p*2*gg* (8); [2] *c*2*mm* (9); [2] *p*4 (10); [2] *p*6 (16)

II Minimal non-isomorphic *klassengleiche* supergroups none

pm No. 3 $p1m1$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	c	1	(1) x,y (2) $\bar{x},y$

I Maximal *translationengleiche* subgroups

[2] $p1$ (1)	1		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$			
pm (3)	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{b}$	
pm (3)	$\langle 2 + (1,0) \rangle$	$2\mathbf{a}, \mathbf{b}$	$1/2, 0$
[2] $\mathbf{b}' = 2\mathbf{b}$			
pg (4)	$\langle 2 + (0,1) \rangle$	$\mathbf{a}, 2\mathbf{b}$	
pm (3)	$\langle 2 \rangle$	$\mathbf{a}, 2\mathbf{b}$	
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
cm (5)	$\langle 2 \rangle$	$2\mathbf{a}, 2\mathbf{b}$	
cm (5)	$\langle 2 + (1,0) \rangle$	$2\mathbf{a}, 2\mathbf{b}$	$1/2, 0$
[3] $\mathbf{a}' = 3\mathbf{a}$			
{ pm (3)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{b}$	
{ pm (3)	$\langle 2 + (2,0) \rangle$	$3\mathbf{a}, \mathbf{b}$	$1, 0$
{ pm (3)	$\langle 2 + (4,0) \rangle$	$3\mathbf{a}, \mathbf{b}$	$2, 0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
pm (3)	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$			
pm (3)	$\langle 2 + (2u,0) \rangle$ $p > 2$; $0 \leq u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}$	$u, 0$
[p] $\mathbf{b}' = p\mathbf{b}$			
pm (3)	$\langle 2 \rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, p\mathbf{b}$	

I Minimal *translationengleiche* supergroups

[2] $p2mm$ (6); [2] $p2mg$ (7)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] cm (5)

- **Decreased unit cell** none

$p1g1$ No. 4 pg

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	a	1	(1) x,y (2) $\bar{x},y+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $p1$ (1) 1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
pg (4)	$\langle 2\rangle$	$2\mathbf{a},\mathbf{b}$	
pg (4)	$\langle 2+(1,0)\rangle$	$2\mathbf{a},\mathbf{b}$	$1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ pg (4)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b}$	
{ pg (4)	$\langle 2+(2,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$1,0$
{ pg (4)	$\langle 2+(4,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$2,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
pg (4)	$\langle 2+(0,1)\rangle$	$\mathbf{a},3\mathbf{b}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
pg (4)	$\langle 2+(2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b}$	$u,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
pg (4)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},p\mathbf{b}$	

I Minimal *translationengleiche* supergroups

[2] $p2mg$ (7); [2] $p2gg$ (8)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] cm (5)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ pm (3)

cm No. 5 *c*1*m*1

Generators selected (1); $t(1,0)$; $t(0,1)$; $t(\frac{1}{2},\frac{1}{2})$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0)+\quad(\frac{1}{2},\frac{1}{2})+$
4	*b*	1	(1) x,y (2) $\bar{x},y$

I Maximal *translationengleiche* subgroups

[2] $c1$ (1, $p1$)	$1+$	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] pg (4)	$1;\ 2+(\frac{1}{2},\frac{1}{2})$		$1/4,0$
[2] pm (3)	$1;\ 2$		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
{ cm (5)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b}$	
{ cm (5)	$\langle 2+(2,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$1,0$
{ cm (5)	$\langle 2+(4,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$2,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
cm (5)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
cm (5)	$\langle 2+(2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b}$	$u,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
cm (5)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},p\mathbf{b}$	

I Minimal *translationengleiche* supergroups

[2] $c2mm$ (9); [3] $p3m1$ (14); [3] $p31m$ (15)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b}$ pm (3)

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	i	1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{x},y$ (4) $x,\bar{y}$

I Maximal *translationengleiche* subgroups

[2] $p1m1$ (3, pm)	1; 3		
[2] $p11m$ (3, pm)	1; 4	$\mathbf{b},-\mathbf{a}$	
[2] $p211$ (2, $p2$)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$p2mg$ (7)	$\langle 2;\ 3+(1,0)\rangle$	$2\mathbf{a},\mathbf{b}$	
$p2mg$ (7)	$\langle 3;\ 2+(1,0)\rangle$	$2\mathbf{a},\mathbf{b}$	$1/2,0$
$p2mm$ (6)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b}$	
$p2mm$ (6)	$\langle(2;\ 3)+(1,0)\rangle$	$2\mathbf{a},\mathbf{b}$	$1/2,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$p2gm$ (7, $p2mg$)	$\langle 2;\ 3+(0,1)\rangle$	$2\mathbf{b},-\mathbf{a}$	
$p2gm$ (7, $p2mg$)	$\langle(2;\ 3)+(0,1)\rangle$	$2\mathbf{b},-\mathbf{a}$	$0,1/2$
$p2mm$ (6)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b}$	
$p2mm$ (6)	$\langle 3;\ 2+(0,1)\rangle$	$\mathbf{a},2\mathbf{b}$	$0,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$c2mm$ (9)	$\langle 2;\ 3\rangle$	$2\mathbf{a},2\mathbf{b}$	
$c2mm$ (9)	$\langle 3;\ 2+(0,1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$0,1/2$
$c2mm$ (9)	$\langle(2;\ 3)+(1,0)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1/2,0$
$c2mm$ (9)	$\langle 2+(1,1);\ 3+(1,0)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1/2,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $p2mm$ (6)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b}$	
{ $p2mm$ (6)	$\langle(2;\ 3)+(2,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$1,0$
{ $p2mm$ (6)	$\langle(2;\ 3)+(4,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$2,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $p2mm$ (6)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b}$	
{ $p2mm$ (6)	$\langle 3;\ 2+(0,2)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,1$
{ $p2mm$ (6)	$\langle 3;\ 2+(0,4)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$p2mm$ (6)	$\langle(2;\ 3)+(2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b}$	$u,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$p2mm$ (6)	$\langle 3;\ 2+(0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b}$	$0,u$

I Minimal *translationengleiche* supergroups

[2] $p4mm$ (11)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $c2mm$ (9)

- **Decreased unit cell** none

$p2mg$ No. 7 $p2mg$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	d	1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{x}+\frac{1}{2},y$ (4) $x+\frac{1}{2},\bar{y}$

I Maximal *translationengleiche* subgroups

[2] $p11g$ (4, pg)	1; 4	$-\mathbf{b},\mathbf{a}$	
[2] $p1m1$ (3, pm)	1; 3		1/4, 0
[2] $p211$ (2, $p2$)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$p2gg$ (8)	$\langle 2;\ 3+(0,1)\rangle$	$\mathbf{a},2\mathbf{b}$	
$p2gg$ (8)	$\langle (2;\ 3)+(0,1)\rangle$	$\mathbf{a},2\mathbf{b}$	$0,1/2$
$p2mg$ (7)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b}$	
$p2mg$ (7)	$\langle 3;\ 2+(0,1)\rangle$	$\mathbf{a},2\mathbf{b}$	$0,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $p2mg$ (7)	$\langle 2;\ 3+(1,0)\rangle$	$3\mathbf{a},\mathbf{b}$	
{ $p2mg$ (7)	$\langle 2+(2,0);\ 3+(3,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$1,0$
{ $p2mg$ (7)	$\langle 2+(4,0);\ 3+(5,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$2,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $p2mg$ (7)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b}$	
{ $p2mg$ (7)	$\langle 3;\ 2+(0,2)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,1$
{ $p2mg$ (7)	$\langle 3;\ 2+(0,4)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$p2mg$ (7)	$\langle 2+(2u,0);\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b}$	$u,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$p2mg$ (7)	$\langle 3;\ 2+(0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b}$	$0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $c2mm$ (9)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $p2mm$ (6)

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	c	1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $p1g1$ (4, pg)	1; 3		$1/4,0$
[2] $p11g$ (4, pg)	1; 4	$-\mathbf{b},\mathbf{a}$	$0,1/4$
[2] $p211$ (2, $p2$)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$

$p2gg$ (8)	$\langle 2;\ 3+(1,0)\rangle$	$3\mathbf{a},\mathbf{b}$	
$p2gg$ (8)	$\langle 2+(2,0);\ 3+(3,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$1,0$
$p2gg$ (8)	$\langle 2+(4,0);\ 3+(5,0)\rangle$	$3\mathbf{a},\mathbf{b}$	$2,0$

[3] $\mathbf{b}'=3\mathbf{b}$

$p2gg$ (8)	$\langle 2;\ 3+(0,1)\rangle$	$\mathbf{a},3\mathbf{b}$	
$p2gg$ (8)	$\langle 2+(0,2);\ 3+(0,1)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,1$
$p2gg$ (8)	$\langle 2+(0,4);\ 3+(0,1)\rangle$	$\mathbf{a},3\mathbf{b}$	$0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$

$p2gg$ (8)	$\langle 2+(2u,0);\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b}$	$u,0$

[p] $\mathbf{b}'=p\mathbf{b}$

$p2gg$ (8)	$\langle 2+(0,2u);\ 3+(0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b}$	$0,u$

I Minimal *translationengleiche* supergroups

[2] $p4gm$ (12)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $c2mm$ (9)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $p2mg$ (7); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $p2gm$ (7, $p2mg$)

$c2mm$ No. 9 $c2mm$

Generators selected (1); $t(1,0)$; $t(0,1)$; $t(\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0)+$ $(\frac{1}{2},\frac{1}{2})+$
8	f	1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{x},y$ (4) $x,\bar{y}$

I Maximal *translationengleiche* subgroups

[2] $c1m1$ (5, cm)	(1; 3)+		
[2] $c11m$ (5, cm)	(1; 4)+	$\mathbf{b}, -\mathbf{a}$	
[2] $c211$ (2, $p2$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $p2gg$ (8)	1; 2; $(3; 4)+(\frac{1}{2},\frac{1}{2})$		
[2] $p2gm$ (7, $p2mg$)	1; 4; $(2; 3)+(\frac{1}{2},\frac{1}{2})$	$\mathbf{b}, -\mathbf{a}$	$1/4, 1/4$
[2] $p2mg$ (7)	1; 3; $(2; 4)+(\frac{1}{2},\frac{1}{2})$		$1/4, 1/4$
[2] $p2mm$ (6)	1; 2; 3; 4		

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$			
{ $c2mm$ (9)	$\langle 2; 3\rangle$	$3\mathbf{a}, \mathbf{b}$	
{ $c2mm$ (9)	$\langle(2; 3)+(2,0)\rangle$	$3\mathbf{a}, \mathbf{b}$	$1, 0$
{ $c2mm$ (9)	$\langle(2; 3)+(4,0)\rangle$	$3\mathbf{a}, \mathbf{b}$	$2, 0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
{ $c2mm$ (9)	$\langle 2; 3\rangle$	$\mathbf{a}, 3\mathbf{b}$	
{ $c2mm$ (9)	$\langle 3; 2+(0,2)\rangle$	$\mathbf{a}, 3\mathbf{b}$	$0, 1$
{ $c2mm$ (9)	$\langle 3; 2+(0,4)\rangle$	$\mathbf{a}, 3\mathbf{b}$	$0, 2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$			
$c2mm$ (9)	$\langle(2; 3)+(2u,0)\rangle$ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}$	$u, 0$
[p] $\mathbf{b}' = p\mathbf{b}$			
$c2mm$ (9)	$\langle 3; 2+(0,2u)\rangle$ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}$	$0, u$

I Minimal *translationengleiche* supergroups

[2] $p4mm$ (11); [2] $p4gm$ (12); [3] $p6mm$ (17)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $p2mm$ (6)

$p4$ No. 10 $p4$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	d	1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{y},x$ (4) $y,\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $p2$ (2)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$

$c4$ (10, $p4$)	$\langle 2;\ 3 \rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}$	
$c4$ (10, $p4$)	$\langle 2+(1,1);\ 3+(1,0) \rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}$	$1/2, 1/2$

- **Series of maximal isomorphic subgroups**

$[p^2]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$p4$ (10)	$\langle 2+(2u,2v);\ 3+(u+v,-u+v) \rangle$ $p > 2$; $0 \le u < p$; $0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3$ (mod 4)	$p\mathbf{a}, p\mathbf{b}$	u,v

$[p = q^2 + r^2]$ $\mathbf{a}' = q\mathbf{a} - r\mathbf{b}$, $\mathbf{b}' = r\mathbf{a} + q\mathbf{b}$

$p4$ (10)	$\langle 2+(2u,0);\ 3+(u,-u) \rangle$ $p > 2$; $q > 0$; $r > 0$; $0 \le u < p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b}, r\mathbf{a}+q\mathbf{b}$	$u,0$

I Minimal *translationengleiche* supergroups

[2] $p4mm$ (11); [2] $p4gm$ (12)

II Minimal non-isomorphic *klassengleiche* supergroups none

$p4mm$ No. 11 $p4mm$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{y},x$	(4) $y,\bar{x}$
			(5) $\bar{x},y$	(6) $x,\bar{y}$	(7) y,x	(8) $\bar{y},\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $p411$ (10, $p4$)	1; 2; 3; 4		
[2] $p21m$ (9, $c2mm$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}$	
[2] $p2m1$ (6, $p2mm$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$

$c4mg$ (12, $p4gm$)	$\langle 2+(1,1);\ 3+(1,0);\ 5+(2,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}$	$1/2, 1/2$
$c4mg$ (12, $p4gm$)	$\langle 2;\ 3;\ 5+(1,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}$	
$c4mm$ (11, $p4mm$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}$	
$c4mm$ (11, $p4mm$)	$\langle 2+(1,1);\ (3;\ 5)+(1,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}$	$1/2, 1/2$

- **Series of maximal isomorphic subgroups**

$[p^2]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$p4mm$ (11)	$\langle 2+(2u,2v);\ 3+(u+v,-u+v);\ 5+(2u,0)\rangle$ $p > 2$; $0 \leq u < p$; $0 \leq v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}$	u, v

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups none

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	d	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{y},x$	(4) $y,\bar{x}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $p411$ (10, $p4$)	1; 2; 3; 4		
[2] $p21m$ (9, $c2mm$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b}$	$0,1/2$
[2] $p2g1$ (8, $p2gg$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$p4gm$ (12)	$\langle 2+(2u,2v);\ 3+(u+v,-u+v);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b}$	u,v

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $c4gm$ (11, $p4mm$)

- **Decreased unit cell** none

$p3$ No. 13 $p3$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
3	d	1	(1) x,y (2) $\bar{y},x-y$ (3) $\bar{x}+y,\bar{x}$

I Maximal *translationengleiche* subgroups

[3] $p1$ (1) 1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$

$h3$ (13, $p3$)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	
$h3$ (13, $p3$)	$\langle 2+(1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	$2/3,1/3$
$h3$ (13, $p3$)	$\langle 2+(1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	$1/3,2/3$

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$

{ $p3$ (13)	$\langle 2\rangle$	$2\mathbf{a},2\mathbf{b}$	
{ $p3$ (13)	$\langle 2+(1,-1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1,0$
{ $p3$ (13)	$\langle 2+(1,2)\rangle$	$2\mathbf{a},2\mathbf{b}$	$0,1$
{ $p3$ (13)	$\langle 2+(2,1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1,1$

- **Series of maximal isomorphic subgroups**

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$p3$ (13)	$\langle 2+(u+v,-u+2v)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b}$	u,v

$[p=q^2+r^2+qr]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$

$p3$ (13)	$\langle 2+(u,-u)\rangle$ $p>6;\ q>0;\ r>0;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b}$	$u,0$

I Minimal *translationengleiche* supergroups

[2] $p3m1$ (14); [2] $p31m$ (15); [2] $p6$ (16)

II Minimal non-isomorphic *klassengleiche* supergroups none

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
6	e	1	(1) x,y (2) $\bar{y},x-y$ (3) $\bar{x}+y,\bar{x}$
			(4) $\bar{y},\bar{x}$ (5) $\bar{x}+y,y$ (6) $x,x-y$

I Maximal *translationengleiche* subgroups

[2] $p311$ (13, $p3$)	1; 2; 3		
[3] $p1m1$ (5, cm)	1; 4	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}$	
[3] $p1m1$ (5, cm)	1; 5	$-\mathbf{a}, -\mathbf{a}-2\mathbf{b}$	
[3] $p1m1$ (5, cm)	1; 6	$-\mathbf{b}, 2\mathbf{a}+\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$

$h3m1$ (15, $p31m$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	
$h3m1$ (15, $p31m$)	$\langle 2+(1,-1);\ 4+(1,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$1,0$
$h3m1$ (15, $p31m$)	$\langle 2+(2,-2);\ 4+(2,2)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$2,0$
$h3m1$ (15, $p31m$)	$\langle 4;\ 2+(0,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$-1/3,1/3$
$h3m1$ (15, $p31m$)	$\langle 2+(1,0);\ 4+(1,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$2/3,1/3$
$h3m1$ (15, $p31m$)	$\langle 2+(2,-1);\ 4+(2,2)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$5/3,1/3$
$h3m1$ (15, $p31m$)	$\langle 4;\ 2+(0,2)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$-2/3,2/3$
$h3m1$ (15, $p31m$)	$\langle (2;\ 4)+(1,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$1/3,2/3$
$h3m1$ (15, $p31m$)	$\langle 2+(2,0);\ 4+(2,2)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}$	$4/3,2/3$

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$

$p3m1$ (14)	$\langle 2;\ 4\rangle$	$2\mathbf{a}, 2\mathbf{b}$	
$p3m1$ (14)	$\langle 2+(1,-1);\ 4+(1,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}$	$1,0$
$p3m1$ (14)	$\langle 2+(1,2);\ 4+(1,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}$	$0,1$
$p3m1$ (14)	$\langle 2+(2,1);\ 4+(2,2)\rangle$	$2\mathbf{a}, 2\mathbf{b}$	$1,1$

- **Series of maximal isomorphic subgroups**

[p^2] $\mathbf{a}'=p\mathbf{a},\ b'=p\mathbf{b}$

$p3m1$ (14)	$\langle 2+(u+v,-u+2v);\ 4+(u+v,u+v)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}$	u,v

I Minimal *translationengleiche* supergroups

[2] $p6mm$ (17)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $h3m1$ (15, $p31m$)

- **Decreased unit cell** none

$p31m$ No. 15 $p31m$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	d	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$
			(4) y,x	(5) $x-y,\bar{y}$	(6) $\bar{x},\bar{x}+y$

I Maximal *translationengleiche* subgroups

[2] $p311$ (13, $p3$)	1; 2; 3		
[3] $p11m$ (5, cm)	1; 4	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b}$	
[3] $p11m$ (5, cm)	1; 5	$\mathbf{a}+2\mathbf{b},-\mathbf{a}$	
[3] $p11m$ (5, cm)	1; 6	$-2\mathbf{a}-\mathbf{b},-\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$h31m$ (14, $p3m1$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$p31m$ (15)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b}$	
$p31m$ (15)	$\langle(2;\ 4)+(1,-1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1,0$
$p31m$ (15)	$\langle 2+(1,2);\ 4+(-1,1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$0,1$
$p31m$ (15)	$\langle 4;\ 2+(2,1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1,1$

- **Series of maximal isomorphic subgroups**

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$p31m$ (15)	$\langle 2+(u+v,-u+2v);\ 4+(u-v,-u+v)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b}$	u,v

I Minimal *translationengleiche* supergroups

[2] $p6mm$ (17)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $h31m$ (14, $p3m1$)

- **Decreased unit cell** none

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	d	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$
			(4) $\bar{x},\bar{y}$	(5) $y,\bar{x}+y$	(6) $x-y,x$

I Maximal *translationengleiche* subgroups

[2] $p3$ (13)	1; 2; 3
[3] $p2$ (2)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$			
{ $h6$ (16, $p6$)	$\langle 2; 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	
{ $h6$ (16, $p6$)	$\langle 2+(1,-1); 4+(2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	1,0
{ $h6$ (16, $p6$)	$\langle 2+(2,-2); 4+(4,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	2,0
[4] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
{ $p6$ (16)	$\langle 2; 4\rangle$	$2\mathbf{a},2\mathbf{b}$	
{ $p6$ (16)	$\langle 2+(1,-1); 4+(2,0)\rangle$	$2\mathbf{a},2\mathbf{b}$	1,0
{ $p6$ (16)	$\langle 2+(1,2); 4+(0,2)\rangle$	$2\mathbf{a},2\mathbf{b}$	0,1
{ $p6$ (16)	$\langle 2+(2,1); 4+(2,2)\rangle$	$2\mathbf{a},2\mathbf{b}$	1,1

- **Series of maximal isomorphic subgroups**

$[p^2]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$			
$p6$ (16)	$\langle 2+(u+v,-u+2v); 4+(2u,2v)\rangle$ $p>1$; $0 \le u < p$; $0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 2$ (mod 3)	$p\mathbf{a},p\mathbf{b}$	u,v
$[p = q^2+r^2+qr]$ $\mathbf{a}' = q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}' = r\mathbf{a}+(q+r)\mathbf{b}$			
$p6$ (16)	$\langle 2+(u,-u); 4+(2u,0)\rangle$ $p>2$; $q>0$; $r>0$; $0 \le u < p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b}$	$u,0$

I Minimal *translationengleiche* supergroups

[2] $p6mm$ (17)

II Minimal non-isomorphic *klassengleiche* supergroups none

$p6mm$ No. 17 $p6mm$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	f	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$
			(4) $\bar{x},\bar{y}$	(5) $y,\bar{x}+y$	(6) $x-y,x$
			(7) $\bar{y},\bar{x}$	(8) $\bar{x}+y,y$	(9) $x,x-y$
			(10) y,x	(11) $x-y,\bar{y}$	(12) $\bar{x},\bar{x}+y$

I Maximal *translationengleiche* subgroups

[2] $p611$ (16, $p6$)	1; 2; 3; 4; 5; 6	
[2] $p31m$ (15)	1; 2; 3; 10; 11; 12	
[2] $p3m1$ (14)	1; 2; 3; 7; 8; 9	
{ [3] $p2mm$ (9, $c2mm$)	1; 4; 7; 10	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b}$
{ [3] $p2mm$ (9, $c2mm$)	1; 4; 8; 11	$\mathbf{a}+2\mathbf{b},-\mathbf{a}$
{ [3] $p2mm$ (9, $c2mm$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$

{ $h6mm$ (17, $p6mm$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	
{ $h6mm$ (17, $p6mm$)	$\langle 2+(1,-1);\ 4+(2,0);\ 7+(1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	$1,0$
{ $h6mm$ (17, $p6mm$)	$\langle 2+(2,-2);\ 4+(4,0);\ 7+(2,2)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b}$	$2,0$

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$

{ $p6mm$ (17)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b}$	
{ $p6mm$ (17)	$\langle 2+(1,-1);\ 4+(2,0);\ 7+(1,1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1,0$
{ $p6mm$ (17)	$\langle 2+(1,2);\ 4+(0,2);\ 7+(1,1)\rangle$	$2\mathbf{a},2\mathbf{b}$	$0,1$
{ $p6mm$ (17)	$\langle 2+(2,1);\ (4;\ 7)+(2,2)\rangle$	$2\mathbf{a},2\mathbf{b}$	$1,1$

- **Series of maximal isomorphic subgroups**

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$p6mm$ (17)	$\langle 2+(u+v,-u+2v);\ 4+(2u,2v);$ $7+(u+v,u+v)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b}$	u,v

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups none

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 1, pp. 78–79.

$P1$ No. 1 $P1$ C_1^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
1	a	1	(1) x,y,z

I Maximal *translationengleiche* subgroups none

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$		
$P1$ (1)	$\langle 1 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$
[2] $\mathbf{b}' = 2\mathbf{b}$		
$P1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$
[2] $\mathbf{c}' = 2\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$
[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$		
$A1$ (1, $P1$)	$\langle 1 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{b}+\mathbf{c}$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$		
$B1$ (1, $P1$)	$\langle 1 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$		
$C1$ (1, $P1$)	$\langle 1 \rangle$	$2\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{c}$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$		
$F1$ (1, $P1$)	$\langle 1 \rangle$	$2\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a}+\mathbf{b}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a}+\mathbf{b}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, 2\mathbf{a}+\mathbf{b}, \mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = \mathbf{a}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = 2\mathbf{a}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, \mathbf{b}, 2\mathbf{a}+\mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a}+\mathbf{b}$, $\mathbf{c}' = \mathbf{a}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a}+\mathbf{b}$, $\mathbf{c}' = \mathbf{a}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, 2\mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a}+\mathbf{b}$, $\mathbf{c}' = 2\mathbf{a}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a}+\mathbf{b}$, $\mathbf{c}' = 2\mathbf{a}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$3\mathbf{a}, 2\mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$
[3] $\mathbf{b}' = 3\mathbf{b}$		
$P1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$
[3] $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = \mathbf{b}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b}+\mathbf{c}$
[3] $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = 2\mathbf{b}+\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, 3\mathbf{b}, 2\mathbf{b}+\mathbf{c}$
[3] $\mathbf{c}' = 3\mathbf{c}$		
$P1$ (1)	$\langle 1 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = q\mathbf{a}+\mathbf{b},\ \mathbf{c}' = r\mathbf{a}+\mathbf{c}$

$P1$ (1)	$\langle 1 \rangle$ $p > 1;\ 0 \le q < p;\ 0 \le r < p$ no conjugate subgroups	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, r\mathbf{a}+\mathbf{c}$

$[p]$ $\mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = q\mathbf{b}+\mathbf{c}$

$P1$ (1)	$\langle 1 \rangle$ $p > 1;\ 0 \le q < p$ no conjugate subgroups	$\mathbf{a}, p\mathbf{b}, q\mathbf{b}+\mathbf{c}$

$[p]$ $\mathbf{c}' = p\mathbf{c}$

$P1$ (1)	$\langle 1 \rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$

I Minimal *translationengleiche* supergroups

[2] $P\bar{1}$ (2); [2] $P121$ (3); [2] $P112$ (3); [2] $P12_11$ (4); [2] $P112_1$ (4); [2] $C121$ (5); [2] $A112$ (5); [2] $P1m1$ (6); [2] $P11m$ (6); [2] $P1c1$ (7); [2] $P11a$ (7); [2] $C1m1$ (8); [2] $A11m$ (8); [2] $C1c1$ (9); [2] $A11a$ (9); [3] $P3$ (143); [3] $P3_1$ (144); [3] $P3_2$ (145); [3] $R3$ (146)

II Minimal non-isomorphic *klassengleiche* supergroups none

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 2, pp. 80–81.

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	i	1	(1) x,y,z (2) $\bar{x},\bar{y},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1) 1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$			
$P\bar{1}$ (2)	$\langle 2 \rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(1,0,0) \rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}' = 2\mathbf{b}$			
$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(0,1,0) \rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{c}' = 2\mathbf{c}$			
$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(0,0,1) \rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$A\bar{1}$ (2, $P\bar{1}$)	$\langle 2 \rangle$	$\mathbf{a},2\mathbf{b},\mathbf{b}+\mathbf{c}$	
$A\bar{1}$ (2, $P\bar{1}$)	$\langle 2+(0,1,0) \rangle$	$\mathbf{a},2\mathbf{b},\mathbf{b}+\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$			
$B\bar{1}$ (2, $P\bar{1}$)	$\langle 2 \rangle$	$2\mathbf{a},\mathbf{b},\mathbf{a}+\mathbf{c}$	
$B\bar{1}$ (2, $P\bar{1}$)	$\langle 2+(1,0,0) \rangle$	$2\mathbf{a},\mathbf{b},\mathbf{a}+\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
$C\bar{1}$ (2, $P\bar{1}$)	$\langle 2 \rangle$	$2\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{1}$ (2, $P\bar{1}$)	$\langle 2+(1,0,0) \rangle$	$2\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$F\bar{1}$ (2, $P\bar{1}$)	$\langle 2 \rangle$	$2\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	
$F\bar{1}$ (2, $P\bar{1}$)	$\langle 2+(1,0,0) \rangle$	$2\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{a}' = 3\mathbf{a}$			
{ $P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2) }	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a}+\mathbf{b}$			
{ $P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2) }	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a}+\mathbf{b}$			
{ $P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a},2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a},2\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2) }	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a},2\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = \mathbf{a}+\mathbf{c}$			
{ $P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{a}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{a}+\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2) }	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{a}+\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = 2\mathbf{a}+\mathbf{c}$			
{ $P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a},\mathbf{b},2\mathbf{a}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a},\mathbf{b},2\mathbf{a}+\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2) }	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a},\mathbf{b},2\mathbf{a}+\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a}+\mathbf{b}$, $\mathbf{c}' = \mathbf{a}+\mathbf{c}$			
{ $P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2) }	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a}+\mathbf{b}$, $\mathbf{c}' = \mathbf{a}+\mathbf{c}$			
{ $P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a},2\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a},2\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2) }	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a},2\mathbf{a}+\mathbf{b},\mathbf{a}+\mathbf{c}$	$2,0,0$

[3] $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2)	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$	$2,0,0$

[3] $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 2\mathbf{a}+\mathbf{b},\ \mathbf{c}' = 2\mathbf{a}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2 \rangle$	$3\mathbf{a}, 2\mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(2,0,0) \rangle$	$3\mathbf{a}, 2\mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$	$1,0,0$
$P\bar{1}$ (2)	$\langle 2+(4,0,0) \rangle$	$3\mathbf{a}, 2\mathbf{a}+\mathbf{b}, 2\mathbf{a}+\mathbf{c}$	$2,0,0$

[3] $\mathbf{b}' = 3\mathbf{b}$

$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(0,2,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,1,0$
$P\bar{1}$ (2)	$\langle 2+(0,4,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,2,0$

[3] $\mathbf{b}' = 3\mathbf{b},\ \mathbf{c}' = \mathbf{b}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(0,2,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b}+\mathbf{c}$	$0,1,0$
$P\bar{1}$ (2)	$\langle 2+(0,4,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b}+\mathbf{c}$	$0,2,0$

[3] $\mathbf{b}' = 3\mathbf{b},\ \mathbf{c}' = 2\mathbf{b}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, 2\mathbf{b}+\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(0,2,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, 2\mathbf{b}+\mathbf{c}$	$0,1,0$
$P\bar{1}$ (2)	$\langle 2+(0,4,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, 2\mathbf{b}+\mathbf{c}$	$0,2,0$

[3] $\mathbf{c}' = 3\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P\bar{1}$ (2)	$\langle 2+(0,0,2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
$P\bar{1}$ (2)	$\langle 2+(0,0,4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = q\mathbf{a}+\mathbf{b},\ \mathbf{c}' = r\mathbf{a}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2+(2u,0,0) \rangle$ $p > 2;\ 0 \le q < p;\ 0 \le r < p;\ 0 \le u < p$ p conjugate subgroups for each triplet of q, r, and prime p	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, r\mathbf{a}+\mathbf{c}$	$u,0,0$

[p] $\mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = q\mathbf{b}+\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2+(0,2u,0) \rangle$ $p > 2;\ 0 \le q < p;\ 0 \le u < p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}, p\mathbf{b}, q\mathbf{b}+\mathbf{c}$	$0,u,0$

[p] $\mathbf{c}' = p\mathbf{c}$

$P\bar{1}$ (2)	$\langle 2+(0,0,2u) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P12/m1$ (10); [2] $P112/m$ (10); [2] $P12_1/m1$ (11); [2] $P112_1/m$ (11); [2] $C12/m1$ (12); [2] $A112/m$ (12); [2] $P12/c1$ (13); [2] $P112/a$ (13); [2] $P12_1/c1$ (14); [2] $P112_1/a$ (14); [2] $C12/c1$ (15); [2] $A112/a$ (15); [3] $P\bar{3}$ (147); [3] $R\bar{3}$ (148)

II Minimal non-isomorphic *klassengleiche* supergroups none

$P2$ No. 3 $P121$ C_2^1

UNIQUE AXIS b

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	e	1	(1) x,y,z (2) $\bar{x},y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1)	1		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}' = 2\mathbf{b}$			
$P12_11$ (4)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$P121$ (3)	$\langle 2\rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
[2] $\mathbf{c}' = 2\mathbf{c}$			
$P121$ (3)	$\langle 2\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P121$ (3)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$			
$P121$ (3)	$\langle 2\rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P121$ (3)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$			
$B121$ (3, $P121$)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	
$B121$ (3, $P121$)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
$C121$ (5)	$\langle 2\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$C121$ (5)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$A121$ (5, $C121$)	$\langle 2\rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a}-2\mathbf{c}$	
$A121$ (5, $C121$)	$\langle 2+(0,0,1)\rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a}-2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$F121$ (5, $C121$)	$\langle 2\rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	
$F121$ (5, $C121$)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
$P121$ (3)	$\langle 2\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
[3] $\mathbf{c}' = 3\mathbf{c}$			
{ $P121$ (3)	$\langle 2\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
{ $P121$ (3)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
{ $P121$ (3)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}' = \mathbf{a}-\mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$			
{ $P121$ (3)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
{ $P121$ (3)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
{ $P121$ (3)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}' = \mathbf{a}-2\mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$			
{ $P121$ (3)	$\langle 2\rangle$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
{ $P121$ (3)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
{ $P121$ (3)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}' = 3\mathbf{a}$			
{ $P121$ (3)	$\langle 2\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
{ $P121$ (3)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1,0,0$
{ $P121$ (3)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$2,0,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{b}' = p\mathbf{b}$			
$P121$ (3)	$\langle 2 \rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	
$[p]$ $\mathbf{a}' = \mathbf{a} - q\mathbf{c},\ \mathbf{c}' = p\mathbf{c}$			
$P121$ (3)	$\langle 2 + (0,0,2u) \rangle$ $p > 2;\ 0 \le q < p;\ 0 \le u < p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a} - q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}' = p\mathbf{a}$			
$P121$ (3)	$\langle 2 + (2u,0,0) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P12/m1$ (10); [2] $P12/c1$ (13); [2] $P222$ (16); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $C222$ (21); [2] $Pmm2$ (25); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pnc2$ (30); [2] $Pba2$ (32); [2] $Pnn2$ (34); [2] $Cmm2$ (35); [2] $Ccc2$ (37); [2] $P4$ (75); [2] $P4_2$ (77); [2] $P\bar{4}$ (81); [3] $P6$ (168); [3] $P6_2$ (171); [3] $P6_4$ (172)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C121$ (5); [2] $A121$ (5, $C121$); [2] $I121$ (5, $C121$)

- **Decreased unit cell** none

(*Continued from the following page*)

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$P112$ (3)	$\langle 2 \rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	
$[p]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = -q\mathbf{a} + \mathbf{b}$			
$P112$ (3)	$\langle 2 + (2u,0,0) \rangle$ $p > 2;\ 0 \le q < p;\ 0 \le u < p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a}, -q\mathbf{a} + \mathbf{b}, \mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
$P112$ (3)	$\langle 2 + (0,2u,0) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0,u,0$

I Minimal *translationengleiche* supergroups

[2] $P112/m$ (10); [2] $P112/a$ (13); [2] $P222$ (16); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $C222$ (21); [2] $Pmm2$ (25); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pnc2$ (30); [2] $Pba2$ (32); [2] $Pnn2$ (34); [2] $Cmm2$ (35); [2] $Ccc2$ (37); [2] $P4$ (75); [2] $P4_2$ (77); [2] $P\bar{4}$ (81); [3] $P6$ (168); [3] $P6_2$ (171); [3] $P6_4$ (172)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A112$ (5); [2] $B112$ (5, $A112$); [2] $I112$ (5, $A112$)

- **Decreased unit cell** none

UNIQUE AXIS c

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	e	1	(1) x,y,z (2) $\bar{x},\bar{y},z$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1)	1		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P112_1$ (4)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P112$ (3)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{a}'=2\mathbf{a}$			
$P112$ (3)	$\langle 2\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112$ (3)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$P112$ (3)	$\langle 2\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P112$ (3)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
$C112$ (3, $P112$)	$\langle 2\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C112$ (3, $P112$)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$A112$ (5)	$\langle 2\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$A112$ (5)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{c}'=2\mathbf{c}$			
$B112$ (5, $A112$)	$\langle 2\rangle$	$-2\mathbf{a}-\mathbf{b},2\mathbf{a},2\mathbf{c}$	
$B112$ (5, $A112$)	$\langle 2+(1,0,0)\rangle$	$-2\mathbf{a}-\mathbf{b},2\mathbf{a},2\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$F112$ (5, $A112$)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{b},2\mathbf{b},2\mathbf{c}$	
$F112$ (5, $A112$)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P112$ (3)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $P112$ (3)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $P112$ (3)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P112$ (3)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-\mathbf{a}+\mathbf{b}$			
{ $P112$ (3)	$\langle 2\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
{ $P112$ (3)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P112$ (3)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
{ $P112$ (3)	$\langle 2\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
{ $P112$ (3)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P112$ (3)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $P112$ (3)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $P112$ (3)	$\langle 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P112$ (3)	$\langle 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$

(*Continued on the preceding page*)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 4, pp. 85–86.

C_2^2 $P\,1\,2_1\,1$ No. 4 $P\,2_1$

UNIQUE AXIS b

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	a	1	(1) x,y,z (2) $\bar{x},y+\frac{1}{2},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1) 1

II Maximal *klassengleiche* subgroups

• **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P12_11$ (4)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P12_11$ (4)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a}$			
$P12_11$ (4)	$\langle 2\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P12_11$ (4)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{c}'=2\mathbf{c}$			
$B12_11$ (4, $P12_11$)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	
$B12_11$ (4, $P12_11$)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P12_11$ (4)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
$P12_11$ (4)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P12_11$ (4)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P12_11$ (4)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$P12_11$ (4)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},3\mathbf{c}$	
$P12_11$ (4)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P12_11$ (4)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$P12_11$ (4)	$\langle 2\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	
$P12_11$ (4)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P12_11$ (4)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P12_11$ (4)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P12_11$ (4)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P12_11$ (4)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$P12_11$ (4)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},p\mathbf{b},\mathbf{c}$	
[p] $\mathbf{a}'=\mathbf{a}-q\mathbf{c}$, $\mathbf{c}'=p\mathbf{c}$			
$P12_11$ (4)	$\langle 2+(0,0,2u)\rangle$ $p>2$; $0\le q<p$; $0\le u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-q\mathbf{c},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$			
$P12_11$ (4)	$\langle 2+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P12_1/m1$ (11); [2] $P12_1/c1$ (14); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $P2_12_12_1$ (19); [2] $C222_1$ (20); [2] $Pmc2_1$ (26); [2] $Pca2_1$ (29); [2] $Pmn2_1$ (31); [2] $Pna2_1$ (33); [2] $Cmc2_1$ (36); [2] $P4_1$ (76); [2] $P4_3$ (78); [3] $P6_1$ (169); [3] $P6_5$ (170); [3] $P6_3$ (173)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations**

[2] $C121$ (5); [2] $A121$ (5, $C121$); [2] $I121$ (5, $C121$)

• **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $P121$ (3)

$P2_1$ No. 4 $P112_1$ C_2^2

UNIQUE AXIS c

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	a	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1)	1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$P112_1$ (4)	$\langle 2\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112_1$ (4)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$P112_1$ (4)	$\langle 2\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P112_1$ (4)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C112_1$ (4, $P112_1$)	$\langle 2\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C112_1$ (4, $P112_1$)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P112_1$ (4)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
$P112_1$ (4)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112_1$ (4)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P112_1$ (4)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b}$			
$P112_1$ (4)	$\langle 2\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$P112_1$ (4)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$P112_1$ (4)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
$P112_1$ (4)	$\langle 2\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$P112_1$ (4)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$P112_1$ (4)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P112_1$ (4)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$P112_1$ (4)	$\langle 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112_1$ (4)	$\langle 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P112_1$ (4)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=-q\mathbf{a}+\mathbf{b}$			
$P112_1$ (4)	$\langle 2+(2u,0,0)\rangle$ $p>2$; $0\le q<p$; $0\le u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a},-q\mathbf{a}+\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$P112_1$ (4)	$\langle 2+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$

I Minimal *translationengleiche* supergroups

[2] $P112_1/m$ (11); [2] $P112_1/a$ (14); [2] $P222_1$ (17); [2] $P2_12_12$ (18); [2] $P2_12_12_1$ (19); [2] $C222_1$ (20); [2] $Pmc2_1$ (26); [2] $Pca2_1$ (29); [2] $Pmn2_1$ (31); [2] $Pna2_1$ (33); [2] $Cmc2_1$ (36); [2] $P4_1$ (76); [2] $P4_3$ (78); [3] $P6_1$ (169); [3] $P6_5$ (170); [3] $P6_3$ (173)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A112$ (5); [2] $B112$ (5, $A112$); [2] $I112$ (5, $A112$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P112$ (3)

C_2^3 $C121$ No. 5 $C2$

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$
4	c	1	(1) x,y,z (2) $\bar{x},y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $C1$ (1, $P1$)	1+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P12_11$ (4)	1; $2+(\frac{1}{2},\frac{1}{2},0)$		1/4, 0, 0
[2] $P121$ (3)	1; 2		

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$C121$ (5)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$C121$ (5)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	0, 0, 1/2
$I121$ (5, $C121$)	$\langle 2\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	
$I121$ (5, $C121$)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	0, 0, 1/2
[3] $\mathbf{b}'=3\mathbf{b}$			
$C121$ (5)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $C121$ (5)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$C121$ (5)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$C121$ (5) }	$\langle 2+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{c},\ \mathbf{c}'=3\mathbf{c}$			
{ $C121$ (5)	$\langle 2\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	
$C121$ (5)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	0, 0, 1
$C121$ (5) }	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{c},\ \mathbf{c}'=3\mathbf{c}$			
{ $C121$ (5)	$\langle 2\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	
$C121$ (5)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	0, 0, 1
$C121$ (5) }	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $C121$ (5)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$C121$ (5)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$C121$ (5) }	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$C121$ (5)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},p\mathbf{b},\mathbf{c}$	
$[p]$ $\mathbf{a}'=\mathbf{a}-2q\mathbf{c},\ \mathbf{c}'=p\mathbf{c}$			
$C121$ (5)	$\langle 2+(0,0,2u)\rangle$ $p>2$; $0\le q<p$; $0\le u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-2q\mathbf{c},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$C121$ (5)	$\langle 2+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $C12/m1$ (12); [2] $C12/c1$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79); [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154); [3] $R32$ (155)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P121$ (3)

 (*Continued from the facing page*)

I Minimal *translationengleiche* supergroups

[2] $A112/m$ (12); [2] $A112/a$ (15); [2] $C222_1$ (20); [2] $C222$ (21); [2] $F222$ (22); [2] $I222$ (23); [2] $I2_12_12_1$ (24); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fmm2$ (42); [2] $Fdd2$ (43); [2] $Imm2$ (44); [2] $Iba2$ (45); [2] $Ima2$ (46); [2] $I4$ (79); [2] $I4_1$ (80); [2] $I\bar{4}$ (82); [3] $P312$ (149); [3] $P321$ (150); [3] $P3_112$ (151); [3] $P3_121$ (152); [3] $P3_212$ (153); [3] $P3_221$ (154); [3] $R32$ (155)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112$ (3)

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$
4	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z$

I Maximal *translationengleiche* subgroups

[2] $A1$ (1, $P1$)	1+	$\mathbf{a}, 1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P112_1$ (4)	1; $2+(0,\frac{1}{2},\frac{1}{2})$		$0,1/4,0$
[2] $P112$ (3)	1; 2		

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$A112$ (5)	$\langle 2\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$A112$ (5)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$I112$ (5, $A112$)	$\langle 2\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$I112$ (5, $A112$)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$A112$ (5)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
$A112$ (5)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$A112$ (5)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$A112$ (5)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
$A112$ (5)	$\langle 2\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$A112$ (5)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$A112$ (5)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-4\mathbf{a}+\mathbf{b}$			
$A112$ (5)	$\langle 2\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	
$A112$ (5)	$\langle 2+(2,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$A112$ (5)	$\langle 2+(4,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$A112$ (5)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$A112$ (5)	$\langle 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$A112$ (5)	$\langle 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$A112$ (5)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=-2q\mathbf{a}+\mathbf{b}$			
$A112$ (5)	$\langle 2+(2u,0,0)\rangle$ $p>2$; $0\le q<p$; $0\le u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a},-2q\mathbf{a}+\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$A112$ (5)	$\langle 2+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$

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International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 6, pp. 90–92.

Pm No. 6 $P1m1$ C_s^1

UNIQUE AXIS b

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	c	1	(1) x,y,z (2) $x,\bar{y},z$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1)	1

II Maximal *klassengleiche* subgroups

● **Enlarged unit cell**

[2] $\mathbf{b}' = 2\mathbf{b}$			
$P1m1$ (6)	$\langle 2 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$P1m1$ (6)	$\langle 2 + (0,1,0) \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0,1/2,0$
[2] $\mathbf{c}' = 2\mathbf{c}$			
$P1c1$ (7)	$\langle 2 + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P1m1$ (6)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
[2] $\mathbf{a}' = 2\mathbf{a}$			
$P1a1$ (7, $P1c1$)	$\langle 2 + (1,0,0) \rangle$	$-2\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{a}$	
$P1m1$ (6)	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$			
$B1e1$ (7, $P1c1$)	$\langle 2 + (0,0,1) \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{c}$	
$B1m1$ (6, $P1m1$)	$\langle 2 \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 2\mathbf{c}$	
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
$C1m1$ (8)	$\langle 2 \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$C1m1$ (8)	$\langle 2 + (0,1,0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0,1/2,0$
[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$A1m1$ (8, $C1m1$)	$\langle 2 \rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a} - 2\mathbf{c}$	
$A1m1$ (8, $C1m1$)	$\langle 2 + (0,1,0) \rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a} - 2\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$F1m1$ (8, $C1m1$)	$\langle 2 \rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a} + \mathbf{c}$	
$F1m1$ (8, $C1m1$)	$\langle 2 + (0,1,0) \rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a} + \mathbf{c}$	$0,1/2,0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
{ $P1m1$ (6)	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
{ $P1m1$ (6)	$\langle 2 + (0,2,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,1,0$
{ $P1m1$ (6)	$\langle 2 + (0,4,0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,2,0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P1m1$ (6)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
[3] $\mathbf{a}' = \mathbf{a} - \mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$			
$P1m1$ (6)	$\langle 2 \rangle$	$\mathbf{a} - \mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
[3] $\mathbf{a}' = \mathbf{a} - 2\mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$			
$P1m1$ (6)	$\langle 2 \rangle$	$\mathbf{a} - 2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
[3] $\mathbf{a}' = 3\mathbf{a}$			
$P1m1$ (6)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	

● **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}' = p\mathbf{b}$			
$P1m1$ (6)	$\langle 2 + (0,2u,0) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0,u,0$
[p] $\mathbf{a}' = \mathbf{a} - q\mathbf{c}$, $\mathbf{c}' = p\mathbf{c}$			
$P1m1$ (6)	$\langle 2 \rangle$ $p > 1$; $0 \le q < p$ no conjugate subgroups	$\mathbf{a} - q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	
[p] $\mathbf{a}' = p\mathbf{a}$			
$P1m1$ (6)	$\langle 2 \rangle$ $p > 1$ no conjugate subgroups	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $P12/m1$ (10); [2] $P12_1/m1$ (11); [2] $Pmm2$ (25); [2] $Pmc2_1$ (26); [2] $Pma2$ (28); [2] $Pmn2_1$ (31); [2] $Amm2$ (38); [2] $Ama2$ (40); [3] $P\bar{6}$ (174)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C1m1$ (8); [2] $A1m1$ (8, $C1m1$); [2] $I1m1$ (8, $C1m1$)

- **Decreased unit cell** none

(*Continued from the following page*)

I Minimal *translationengleiche* supergroups

[2] $P112/m$ (10); [2] $P112_1/m$ (11); [2] $Pmm2$ (25); [2] $Pmc2_1$ (26); [2] $Pma2$ (28); [2] $Pmn2_1$ (31); [2] $Amm2$ (38); [2] $Ama2$ (40); [3] $P\bar{6}$ (174)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A11m$ (8); [2] $B11m$ (8, $A11m$); [2] $I11m$ (8, $A11m$)

- **Decreased unit cell** none

Pm No. 6 $P11m$ C_s^1

UNIQUE AXIS c

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	c	1	(1) x,y,z (2) $x,y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1) 1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P11m$ (6)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P11m$ (6)	$\langle 2 + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$			
$P11a$ (7)	$\langle 2 + (1,0,0) \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P11m$ (6)	$\langle 2 \rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
[2] $\mathbf{b}' = 2\mathbf{b}$			
$P11b$ (7, $P11a$)	$\langle 2 + (0,1,0) \rangle$	$2\mathbf{b}, -\mathbf{a} - 2\mathbf{b}, \mathbf{c}$	
$P11m$ (6)	$\langle 2 \rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
$C11e$ (7, $P11a$)	$\langle 2 + (1,0,0) \rangle$	$2\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$	
$C11m$ (6, $P11m$)	$\langle 2 \rangle$	$2\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$	
[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$A11m$ (8)	$\langle 2 \rangle$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	
$A11m$ (8)	$\langle 2 + (0,0,1) \rangle$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$			
$B11m$ (8, $A11m$)	$\langle 2 \rangle$	$-2\mathbf{a} - \mathbf{b}, 2\mathbf{a}, 2\mathbf{c}$	
$B11m$ (8, $A11m$)	$\langle 2 + (0,0,1) \rangle$	$-2\mathbf{a} - \mathbf{b}, 2\mathbf{a}, 2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$F11m$ (8, $A11m$)	$\langle 2 \rangle$	$\mathbf{a} - \mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	
$F11m$ (8, $A11m$)	$\langle 2 + (0,0,1) \rangle$	$\mathbf{a} - \mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}' = 3\mathbf{c}$			
{ $P11m$ (6)	$\langle 2 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
{ $P11m$ (6)	$\langle 2 + (0,0,2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
{ $P11m$ (6)	$\langle 2 + (0,0,4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}' = 3\mathbf{a}$			
$P11m$ (6)	$\langle 2 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$			
$P11m$ (6)	$\langle 2 \rangle$	$3\mathbf{a}, -\mathbf{a} + \mathbf{b}, \mathbf{c}$	
[3] $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -2\mathbf{a} + \mathbf{b}$			
$P11m$ (6)	$\langle 2 \rangle$	$3\mathbf{a}, -2\mathbf{a} + \mathbf{b}, \mathbf{c}$	
[3] $\mathbf{b}' = 3\mathbf{b}$			
$P11m$ (6)	$\langle 2 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P11m$ (6)	$\langle 2 + (0,0,2u) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = -q\mathbf{a} + \mathbf{b}$			
$P11m$ (6)	$\langle 2 \rangle$ $p > 1$; $0 \le q < p$ no conjugate subgroups	$p\mathbf{a}, -q\mathbf{a} + \mathbf{b}, \mathbf{c}$	
[p] $\mathbf{b}' = p\mathbf{b}$			
$P11m$ (6)	$\langle 2 \rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	

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International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 7, pp. 93–94.

C_s^2 $P1c1$ No. 7 Pc

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	a	1	(1) x,y,z (2) $x,\bar{y},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1)	1		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$P1c1$ (7)	$\langle 2\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P1c1$ (7)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a}$			
$P1c1$ (7)	$\langle 2\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P1n1$ (7, $P1c1$)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	
[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
$C1c1$ (9)	$\langle 2\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$C1c1$ (9)	$\langle 2+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $P1c1$ (7)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $P1c1$ (7)	$\langle 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P1c1$ (7)	$\langle 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P1c1$ (7)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
$P1c1$ (7)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{c}'=-2\mathbf{a}+\mathbf{c}$			
$P1c1$ (7)	$\langle 2+(-1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{c}'=-4\mathbf{a}+\mathbf{c}$			
$P1c1$ (7)	$\langle 2+(-2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-4\mathbf{a}+\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$P1c1$ (7)	$\langle 2+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$P1c1$ (7)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{c}'=-2q\mathbf{a}+\mathbf{c}$			
$P1c1$ (7)	$\langle 2+(-q,0,0)\rangle$ $p>1$; $0\le q<p$ no conjugate subgroups	$p\mathbf{a},\mathbf{b},-2q\mathbf{a}+\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $P12/c1$ (13); [2] $P12_1/c1$ (14); [2] $Pmc2_1$ (26); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pca2_1$ (29); [2] $Pnc2$ (30); [2] $Pmn2_1$ (31); [2] $Pba2$ (32); [2] $Pna2_1$ (33); [2] $Pnn2$ (34); [2] $Aem2$ (39); [2] $Aea2$ (41)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C1c1$ (9); [2] $A1m1$ (8, $C1m1$); [2] $I1c1$ (9, $C1c1$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P1m1$ (6)

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
2	a	1	(1) x,y,z (2) $x+\frac{1}{2},y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P1$ (1) 1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P11a$ (7)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P11a$ (7)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{b}'=2\mathbf{b}$			
$P11a$ (7)	$\langle 2\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P11n$ (7, $P11a$)	$\langle 2+(0,1,0)\rangle$	$\mathbf{a}-2\mathbf{b},2\mathbf{b},\mathbf{c}$	
[2] $\mathbf{b}'=2\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$A11a$ (9)	$\langle 2\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$A11a$ (9)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$\{$ $P11a$ (7)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P11a$ (7)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P11a$ (7)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P11a$ (7)	$\langle 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
[3] $\mathbf{b}'=3\mathbf{b}$			
$P11a$ (7)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{b}$, $\mathbf{b}'=3\mathbf{b}$			
$P11a$ (7)	$\langle 2+(0,-1,0)\rangle$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{b}$, $\mathbf{b}'=3\mathbf{b}$			
$P11a$ (7)	$\langle 2+(0,-2,0)\rangle$	$\mathbf{a}-4\mathbf{b},3\mathbf{b},\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P11a$ (7)	$\langle 2+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$			
$P11a$ (7)	$\langle 2+(\frac{p}{2}-\frac{1}{2}),0,0\rangle$ $p>2$ no conjugate subgroups	$p\mathbf{a},\mathbf{b},\mathbf{c}$	
[p] $\mathbf{a}'=\mathbf{a}-2q\mathbf{b}$, $\mathbf{b}'=p\mathbf{b}$			
$P11a$ (7)	$\langle 2+(0,-q,0)\rangle$ $p>1$; $0\le q<p$ no conjugate subgroups	$\mathbf{a}-2q\mathbf{b},p\mathbf{b},\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $P112/a$ (13); [2] $P112_1/a$ (14); [2] $Pmc2_1$ (26); [2] $Pcc2$ (27); [2] $Pma2$ (28); [2] $Pca2_1$ (29); [2] $Pnc2$ (30); [2] $Pmn2_1$ (31); [2] $Pba2$ (32); [2] $Pna2_1$ (33); [2] $Pnn2$ (34); [2] $Aem2$ (39); [2] $Aea2$ (41)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A11a$ (9); [2] $B11m$ (8, $A11m$); [2] $I11a$ (9, $A11a$)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $P11m$ (6)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 8, pp. 95–96.

C_s^3 $C1m1$ No. 8 Cm

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$
4	b	1	(1) x,y,z (2) $x,\bar{y},z$

I Maximal *translationengleiche* subgroups

[2] $C1$ (1, $P1$)	$1+$	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P1a1$ (7, $P1c1$)	1; $2+(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	$0,1/4,0$
[2] $P1m1$ (6)	1; 2		

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$C1c1$ (9)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$I1c1$ (9, $C1c1$)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	
$C1m1$ (8)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$I1m1$ (8, $C1m1$)	$\langle 2\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $C1m1$ (8)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $C1m1$ (8)	$\langle 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $C1m1$ (8)	$\langle 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$C1m1$ (8)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$C1m1$ (8)	$\langle 2\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$C1m1$ (8)	$\langle 2\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
$C1m1$ (8)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$C1m1$ (8)	$\langle 2+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{a}'=\mathbf{a}-2q\mathbf{c}$, $\mathbf{c}'=p\mathbf{c}$			
$C1m1$ (8)	$\langle 2\rangle$ $p>1$; $0\le q<p$ no conjugate subgroups	$\mathbf{a}-2q\mathbf{c},\mathbf{b},p\mathbf{c}$	
[p] $\mathbf{a}'=p\mathbf{a}$			
$C1m1$ (8)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$p\mathbf{a},\mathbf{b},\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $C12/m1$ (12); [2] $Cmm2$ (35); [2] $Cmc2_1$ (36); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Fmm2$ (42); [2] $Imm2$ (44); [2] $Ima2$ (46); [3] $P3m1$ (156); [3] $P31m$ (157); [3] $R3m$ (160)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $P1m1$ (6)

Cm No. 8 $A11m$ C_s^3

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$
4	b	1	(1) x,y,z (2) $x,y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $A1$ (1, $P1$)	1+	$\mathbf{a}, 1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P11b$ (7, $P11a$)	1; $2+(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$	$0,0,1/4$
[2] $P11m$ (6)	1; 2		

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$A11a$ (9)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$I11a$ (9, $A11a$)	$\langle 2+(1,0,0)\rangle$	$2\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	
$A11m$ (8)	$\langle 2\rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$I11m$ (8, $A11m$)	$\langle 2\rangle$	$2\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $A11m$ (8)	$\langle 2\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
{ $A11m$ (8)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
{ $A11m$ (8)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$A11m$ (8)	$\langle 2\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=-4\mathbf{a}+\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$	$3\mathbf{a}, -4\mathbf{a}+\mathbf{b}, \mathbf{c}$	
[3] $\mathbf{b}'=3\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$A11m$ (8)	$\langle 2+(0,0,2u)\rangle$ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=-2q\mathbf{a}+\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$ $p>1$; $0 \le q < p$ no conjugate subgroups	$p\mathbf{a}, -2q\mathbf{a}+\mathbf{b}, \mathbf{c}$	
[p] $\mathbf{b}'=p\mathbf{b}$			
$A11m$ (8)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $A112/m$ (12); [2] $Cmm2$ (35); [2] $Cmc2_1$ (36); [2] $Amm2$ (38); [2] $Aem2$ (39); [2] $Fmm2$ (42); [2] $Imm2$ (44); [2] $Ima2$ (46); [3] $P3m1$ (156); [3] $P31m$ (157); [3] $R3m$ (160)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P11m$ (6)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 9, pp. 97–98.

C_s^4 $\quad C1c1 \quad$ No. 9 $\quad Cc$

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$
4	a	1	(1) x,y,z (2) $x,\bar{y},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $C1$ (1, $P1$)	1+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P1c1$ (7)	1; 2		
[2] $P1n1$ (7, $P1c1$)	1; $2+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{a},\mathbf{b},-\mathbf{a}+\mathbf{c}$	0, 1/4, 0

- **Enlarged unit cell**

[3] $\mathbf{b}'=3\mathbf{b}$			
$\{$ $C1c1$ (9)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$C1c1$ (9)	$\langle 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$C1c1$ (9)	$\langle 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$C1c1$ (9)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{c},\ \mathbf{c}'=3\mathbf{c}$			
$C1c1$ (9)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{c},\ \mathbf{c}'=3\mathbf{c}$			
$C1c1$ (9)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
$C1c1$ (9)	$\langle 2\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$C1c1$ (9)	$\langle 2+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{a}'=\mathbf{a}-2q\mathbf{c},\ \mathbf{c}'=p\mathbf{c}$			
$C1c1$ (9)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$; $0\le q<p$ no conjugate subgroups	$\mathbf{a}-2q\mathbf{c},\mathbf{b},p\mathbf{c}$	
$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$C1c1$ (9)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$p\mathbf{a},\mathbf{b},\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $C12/c1$ (15); [2] $Cmc2_1$ (36); [2] $Ccc2$ (37); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fdd2$ (43); [2] $Iba2$ (45); [2] $Ima2$ (46); [3] $P3c1$ (158); [3] $P31c$ (159); [3] $R3c$ (161)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $F1m1$ (8, $C1m1$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C1m1$ (8); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b}$ $P1c1$ (7)

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$
4	a	1	(1) x,y,z (2) $x+\frac{1}{2},y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $A1$ (1, $P1$)	1+	$\mathbf{a}, 1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P11a$ (7)	1; 2		
[2] $P11n$ (7, $P11a$)	1; $2+(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{a}-\mathbf{b},\mathbf{b},\mathbf{c}$	$0,0,1/4$

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
{ $A11a$ (9)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $A11a$ (9)	$\langle 2+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $A11a$ (9)	$\langle 2+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$A11a$ (9)	$\langle 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
$A11a$ (9)	$\langle 2+(1,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-4\mathbf{a}+\mathbf{b}$			
$A11a$ (9)	$\langle 2+(1,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	
[3] $\mathbf{b}'=3\mathbf{b}$			
$A11a$ (9)	$\langle 2\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$A11a$ (9)	$\langle 2+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=-2q\mathbf{a}+\mathbf{b}$			
$A11a$ (9)	$\langle 2+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2$; $0\le q<p$ no conjugate subgroups	$p\mathbf{a},-2q\mathbf{a}+\mathbf{b},\mathbf{c}$	
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$A11a$ (9)	$\langle 2\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},p\mathbf{b},\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $A112/a$ (15); [2] $Cmc2_1$ (36); [2] $Ccc2$ (37); [2] $Ama2$ (40); [2] $Aea2$ (41); [2] $Fdd2$ (43); [2] $Iba2$ (45); [2] $Ima2$ (46); [3] $P3c1$ (158); [3] $P31c$ (159); [3] $R3c$ (161)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $F11m$ (8, $A11m$)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $A11m$ (8); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P11a$ (7)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 10, pp. 99–102.

C_{2h}^1 $P12/m1$ No. 10 $P2/m$

UNIQUE AXIS b

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	o	1	(1) x,y,z (2) $\bar{x},y,\bar{z}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y},z$

I Maximal *translationengleiche* subgroups

[2] $P1m1$ (6)	1; 4
[2] $P121$ (3)	1; 2
[2] $P\bar{1}$ (2)	1; 3

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}' = 2\mathbf{b}$			
$P12_1/m1$ (11)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0,1/2,0$
$P12/m1$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$P12/m1$ (10)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0,1/2,0$
[2] $\mathbf{c}' = 2\mathbf{c}$			
$P12/c1$ (13)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P12/c1$ (13)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
$P12/m1$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P12/m1$ (10)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a}$			
$P12/a1$ (13, $P12/c1$)	$\langle 3;\ 2+(1,0,0)\rangle$	$-2\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{a}$	
$P12/a1$ (13, $P12/c1$)	$\langle 2;\ 3+(1,0,0)\rangle$	$-2\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{a}$	$1/2,0,0$
$P12/m1$ (10)	$\langle 2;\ 3\rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P12/m1$ (10)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{c}' = 2\mathbf{c}$			
$B12/e1$ (13, $P12/c1$)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	
$B12/e1$ (13, $P12/c1$)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
$B12/m1$ (10, $P12/m1$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	
$B12/m1$ (10, $P12/m1$)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$C12/m1$ (12)	$\langle 2;\ 3\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
$C12/m1$ (12)	$\langle 2;\ 3+(0,1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0,1/2,0$
$C12/m1$ (12)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2,0,0$
$C12/m1$ (12)	$\langle 2+(1,0,0);\ 3+(1,1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$A12/m1$ (12, $C12/m1$)	$\langle 2;\ 3\rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a}-2\mathbf{c}$	
$A12/m1$ (12, $C12/m1$)	$\langle (2;\ 3)+(0,0,1)\rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a}-2\mathbf{c}$	$0,0,1/2$
$A12/m1$ (12, $C12/m1$)	$\langle 2;\ 3+(0,1,0)\rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a}-2\mathbf{c}$	$0,1/2,0$
$A12/m1$ (12, $C12/m1$)	$\langle 2+(0,0,1);\ 3+(0,1,1)\rangle$	$2\mathbf{c}, 2\mathbf{b}, -\mathbf{a}-2\mathbf{c}$	$0,1/2,1/2$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$F12/m1$ (12, $C12/m1$)	$\langle 2;\ 3\rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	
$F12/m1$ (12, $C12/m1$)	$\langle 2;\ 3+(0,1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$0,1/2,0$
$F12/m1$ (12, $C12/m1$)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$1/2,0,0$
$F12/m1$ (12, $C12/m1$)	$\langle 2+(1,0,0);\ 3+(1,1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
{ $P12/m1$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
{ $P12/m1$ (10)	$\langle 2;\ 3+(0,2,0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,1,0$
{ $P12/m1$ (10)	$\langle 2;\ 3+(0,4,0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,2,0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
{ $P12/m1$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
{ $P12/m1$ (10)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
{ $P12/m1$ (10)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}' = \mathbf{a}-\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$			
{ $P12/m1$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
{ $P12/m1$ (10)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
{ $P12/m1$ (10)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$

[3] $\mathbf{a}' = \mathbf{a} - 2\mathbf{c},\ \mathbf{c}' = 3\mathbf{c}$			
$P12/m1$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	
$P12/m1$ (10)	$\langle (2;\ 3) + (0,0,2)\rangle$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,1$
$P12/m1$ (10)	$\langle (2;\ 3) + (0,0,4)\rangle$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}' = 3\mathbf{a}$			
$P12/m1$ (10)	$\langle 2;\ 3\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$P12/m1$ (10)	$\langle (2;\ 3) + (2,0,0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1,0,0$
$P12/m1$ (10)	$\langle (2;\ 3) + (4,0,0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$2,0,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{b}' = p\mathbf{b}$			
$P12/m1$ (10)	$\langle 2;\ 3 + (0,2u,0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{a}' = \mathbf{a} - q\mathbf{c},\ \mathbf{c}' = p\mathbf{c}$			
$P12/m1$ (10)	$\langle (2;\ 3) + (0,0,2u)\rangle$ $p > 2;\ 0 \leq q < p;\ 0 \leq u < p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}' = p\mathbf{a}$			
$P12/m1$ (10)	$\langle (2;\ 3) + (2u,0,0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] *Pmmm* (47); [2] *Pccm* (49); [2] *Pmma* (51); [2] *Pmna* (53); [2] *Pbam* (55); [2] *Pnnm* (58); [2] *Cmmm* (65); [2] *Cccm* (66); [2] $P4/m$ (83); [2] $P4_2/m$ (84); [3] $P6/m$ (175)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C12/m1$ (12); [2] $A12/m1$ (12, $C12/m1$); [2] $I12/m1$ (12, $C12/m1$)

- **Decreased unit cell** none

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	o	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P11m$ (6)	1; 4
[2] $P112$ (3)	1; 2
[2] $P\bar{1}$ (2)	1; 3

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P112_1/m$ (11)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P112_1/m$ (11)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P112/m$ (10)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a}$			
$P112/a$ (13)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112/a$ (13)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112/m$ (10)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$P112/b$ (13, $P112/a$)	$\langle 3;\ 2+(0,1,0)\rangle$	$2\mathbf{b},-\mathbf{a}-2\mathbf{b},\mathbf{c}$	
$P112/b$ (13, $P112/a$)	$\langle 2;\ 3+(0,1,0)\rangle$	$2\mathbf{b},-\mathbf{a}-2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P112/m$ (10)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C112/e$ (13, $P112/a$)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C112/e$ (13, $P112/a$)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C112/m$ (10, $P112/m$)	$\langle 2;\ 3\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C112/m$ (10, $P112/m$)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$A112/m$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$A112/m$ (12)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$A112/m$ (12)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$A112/m$ (12)	$\langle 2+(0,1,0);\ 3+(0,1,1)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{c}'=2\mathbf{c}$			
$B112/m$ (12, $A112/m$)	$\langle 2;\ 3\rangle$	$-2\mathbf{a}-\mathbf{b},2\mathbf{a},2\mathbf{c}$	
$B112/m$ (12, $A112/m$)	$\langle (2;\ 3)+(1,0,0)\rangle$	$-2\mathbf{a}-\mathbf{b},2\mathbf{a},2\mathbf{c}$	$1/2,0,0$
$B112/m$ (12, $A112/m$)	$\langle 2;\ 3+(0,0,1)\rangle$	$-2\mathbf{a}-\mathbf{b},2\mathbf{a},2\mathbf{c}$	$0,0,1/2$
$B112/m$ (12, $A112/m$)	$\langle 2+(1,0,0);\ 3+(1,0,1)\rangle$	$-2\mathbf{a}-\mathbf{b},2\mathbf{a},2\mathbf{c}$	$1/2,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F112/m$ (12, $A112/m$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},2\mathbf{b},2\mathbf{c}$	
$F112/m$ (12, $A112/m$)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},2\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F112/m$ (12, $A112/m$)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$F112/m$ (12, $A112/m$)	$\langle 2+(0,1,0);\ 3+(0,1,1)\rangle$	$\mathbf{a}-\mathbf{b},2\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P112/m$ (10)	$\langle 2;\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P112/m$ (10)	$\langle 2;\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112/m$ (10)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P112/m$ (10)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b}$			
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$P112/m$ (10)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$P112/m$ (10)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$

[3] $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = -2\mathbf{a}+\mathbf{b}$			
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	
$P112/m$ (10)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$1,0,0$
$P112/m$ (10)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$2,0,0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
$P112/m$ (10)	$\langle 2;\ 3\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
$P112/m$ (10)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,1,0$
$P112/m$ (10)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0,2,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P112/m$ (10)	$\langle 2;\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = -q\mathbf{a}+\mathbf{b}$			
$P112/m$ (10)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a}, -q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$u,0,0$
[p] $\mathbf{b}' = p\mathbf{b}$			
$P112/m$ (10)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0,u,0$

I Minimal *translationengleiche* supergroups

[2] *Pmmm* (47); [2] *Pccm* (49); [2] *Pmma* (51); [2] *Pmna* (53); [2] *Pbam* (55); [2] *Pnnm* (58); [2] *Cmmm* (65); [2] *Cccm* (66); [2] $P4/m$ (83); [2] $P4_2/m$ (84); [3] $P6/m$ (175)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A112/m$ (12); [2] $B112/m$ (12, $A112/m$); [2] $I112/m$ (12, $A112/m$)

- **Decreased unit cell** none

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 11, pp. 103–105.

C_{2h}^2 $P\,1\,2_1/m\,1$ No. 11 $P\,2_1/m$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	f	1	(1) x,y,z (2) $\bar{x},y+\frac{1}{2},\bar{z}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y}+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P1m1$ (6)	1; 4		$0,1/4,0$
[2] $P12_11$ (4)	1; 2		
[2] $P\bar{1}$ (2)	1; 3		

II Maximal *klassengleiche* subgroups

• **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P12_1/c1$ (14)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P12_1/c1$ (14)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P12_1/m1$ (11)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a}$			
$P12_1/a1$ (14, $P12_1/c1$)	$\langle 3;\ 2+(1,0,0)\rangle$	$-2\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{a}$	
$P12_1/a1$ (14, $P12_1/c1$)	$\langle 2;\ 3+(1,0,0)\rangle$	$-2\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{a}$	$1/2,0,0$
$P12_1/m1$ (11)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P12_1/m1$ (11)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{c}'=2\mathbf{c}$			
$B12_1/e1$ (14, $P12_1/c1$)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	
$B12_1/e1$ (14, $P12_1/c1$)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$B12_1/m1$ (11, $P12_1/m1$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	
$B12_1/m1$ (11, $P12_1/m1$)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $P12_1/m1$ (11)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $P12_1/m1$ (11)	$\langle 2+(0,1,0);\ 3+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P12_1/m1$ (11)	$\langle 2+(0,1,0);\ 3+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P12_1/m1$ (11)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{c},\ \mathbf{c}'=3\mathbf{c}$			
{ $P12_1/m1$ (11)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},3\mathbf{c}$	
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{c},\ \mathbf{c}'=3\mathbf{c}$			
{ $P12_1/m1$ (11)	$\langle 2;\ 3\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $P12_1/m1$ (11)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P12_1/m1$ (11)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$P12_1/m1$ (11)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2},0);\ 3+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{a}'=\mathbf{a}-q\mathbf{c},\ \mathbf{c}'=p\mathbf{c}$			
$P12_1/m1$ (11)	$\langle (2;\ 3)+(0,0,2u)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-q\mathbf{c},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$			
$P12_1/m1$ (11)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] *Pmma* (51); [2] *Pbcm* (57); [2] *Pmmn* (59); [2] *Pnma* (62); [2] *Cmcm* (63); [3] $P6_3/m$ (176)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C12/m1$ (12); [2] $A12/m1$ (12, $C12/m1$); [2] $I12/m1$ (12, $C12/m1$)

- **Decreased unit cell**

[2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P12/m1$ (10)

$P2_1/m$ UNIQUE AXIS c No. 11

(*Continued from the facing page*)

I Minimal *translationengleiche* supergroups

[2] *Pmma* (51); [2] *Pbcm* (57); [2] *Pmmn* (59); [2] *Pnma* (62); [2] *Cmcm* (63); [3] $P6_3/m$ (176)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A112/m$ (12); [2] $B112/m$ (12, $A112/m$); [2] $I112/m$ (12, $A112/m$)

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112/m$ (10)

UNIQUE AXIS c

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	f	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,y,\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P11m$ (6)	1; 4	$0,0,1/4$
[2] $P112_1$ (4)	1; 2	
[2] $P\bar{1}$ (2)	1; 3	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$P112_1/a$ (14)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112_1/a$ (14)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$P112_1/m$ (11)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112_1/m$ (11)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$P112_1/b$ (14, $P112_1/a$)	$\langle 3;\ 2+(0,1,0)\rangle$	$2\mathbf{b},-\mathbf{a}-2\mathbf{b},\mathbf{c}$	
$P112_1/b$ (14, $P112_1/a$)	$\langle 2;\ 3+(0,1,0)\rangle$	$2\mathbf{b},-\mathbf{a}-2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$P112_1/m$ (11)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P112_1/m$ (11)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C112_1/e$ (14, $P112_1/a$)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C112_1/e$ (14, $P112_1/a$)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C112_1/m$ (11, $P112_1/m$)	$\langle 2;\ 3\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C112_1/m$ (11, $P112_1/m$)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P112_1/m$ (11)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P112_1/m$ (11)	$\langle 2+(0,0,1);\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P112_1/m$ (11)	$\langle 2+(0,0,1);\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P112_1/m$ (11)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112_1/m$ (11)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P112_1/m$ (11)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b}$			
$P112_1/m$ (11)	$\langle 2;\ 3\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	
$P112_1/m$ (11)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$P112_1/m$ (11)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
$P112_1/m$ (11)	$\langle 2;\ 3\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$P112_1/m$ (11)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$P112_1/m$ (11)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P112_1/m$ (11)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$P112_1/m$ (11)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112_1/m$ (11)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P112_1/m$ (11)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=-q\mathbf{a}+\mathbf{b}$			
$P112_1/m$ (11)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2;\ 0\leq q<p;\ 0\leq u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a},-q\mathbf{a}+\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$P112_1/m$ (11)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$

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$C2/m$ No. 12 $C12/m1$ C_{2h}^3

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$
8 j 1	(1) x,y,z (2) $\bar{x},y,\bar{z}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y},z$

I Maximal *translationengleiche* subgroups

[2] $C1m1$ (8)	(1; 4)+		
[2] $C121$ (5)	(1; 2)+		
[2] $C\bar{1}$ (2, $P\bar{1}$)	(1; 3)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P12_1/a1$ (14, $P12_1/c1$)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] $P12/a1$ (13, $P12/c1$)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$1/4,1/4,0$
[2] $P12_1/m1$ (11)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$1/4,1/4,0$
[2] $P12/m1$ (10)	1; 2; 3; 4		

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$C12/c1$ (15)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$C12/c1$ (15)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$I12/c1$ (15, $C12/c1$)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	
$I12/c1$ (15, $C12/c1$)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$C12/m1$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$I12/m1$ (12, $C12/m1$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	
$I12/m1$ (12, $C12/m1$)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{b}'=3\mathbf{b}$			
$C12/m1$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$C12/m1$ (12)	$\langle 2;\ 3+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$C12/m1$ (12)	$\langle 2;\ 3+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$C12/m1$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$C12/m1$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$C12/m1$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,2)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,4)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$C12/m1$ (12)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$C12/m1$ (12)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$C12/m1$ (12)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$C12/m1$ (12)	$\langle 2;\ 3+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{a}'=\mathbf{a}-2q\mathbf{c}$, $\mathbf{c}'=p\mathbf{c}$			
$C12/m1$ (12)	$\langle (2;\ 3)+(0,0,2u)\rangle$ $p>2$; $0\le q<p$; $0\le u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-2q\mathbf{c},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$			
$C12/m1$ (12)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] *Cmcm* (63); [2] *Cmce* (64); [2] *Cmmm* (65); [2] *Cmme* (67); [2] *Fmmm* (69); [2] *Immm* (71); [2] *Ibam* (72); [2] *Imma* (74); [2] $I4/m$ (87); [3] $P\bar{3}12/m$ (162, $P\bar{3}1m$); [3] $P\bar{3}2/m1$ (164, $P\bar{3}m1$); [3] $R\bar{3}2/m$ (166, $R\bar{3}m$)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P12/m1$ (10)

I Minimal *translationengleiche* supergroups

[2] *Cmcm* (63); [2] *Cmce* (64); [2] *Cmmm* (65); [2] *Cmme* (67); [2] *Fmmm* (69); [2] *Immm* (71); [2] *Ibam* (72); [2] *Imma* (74); [2] $I4/m$ (87); [3] $P\bar{3}12/m$ (162, $P\bar{3}1m$); [3] $P\bar{3}2/m1$ (164, $P\bar{3}m1$); [3] $R\bar{3}2/m$ (166, $R\bar{3}m$)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112/m$ (10)

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+$
8 j 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $A11m$ (8)	(1; 4)+		
[2] $A112$ (5)	(1; 2)+		
[2] $A\bar{1}$ (2, $P\bar{1}$)	(1; 3)+	$\mathbf{a},1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P112_1/b$ (14, $P112_1/a$)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P112/b$ (13, $P112/a$)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	0, 1/4, 1/4
[2] $P112_1/m$ (11)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	0, 1/4, 1/4
[2] $P112/m$ (10)	1; 2; 3; 4		

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$A112/a$ (15)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$A112/a$ (15)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	1/2, 0, 0
$I112/a$ (15, $A112/a$)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$I112/a$ (15, $A112/a$)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	1/2, 0, 0
$A112/m$ (12)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$A112/m$ (12)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	1/2, 0, 0
$I112/m$ (12, $A112/m$)	$\langle 2;\ 3\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$I112/m$ (12, $A112/m$)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	1/2, 0, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $A112/m$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $A112/m$ (12)	$\langle 2;\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
{ $A112/m$ (12)	$\langle 2;\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $A112/m$ (12)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $A112/m$ (12)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
{ $A112/m$ (12)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
{ $A112/m$ (12)	$\langle 2;\ 3\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
{ $A112/m$ (12)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	1, 0, 0
{ $A112/m$ (12)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-4\mathbf{a}+\mathbf{b}$			
{ $A112/m$ (12)	$\langle 2;\ 3\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	
{ $A112/m$ (12)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	1, 0, 0
{ $A112/m$ (12)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $A112/m$ (12)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $A112/m$ (12)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
{ $A112/m$ (12)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$A112/m$ (12)	$\langle 2;\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=-2q\mathbf{a}+\mathbf{b}$			
$A112/m$ (12)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a},-2q\mathbf{a}+\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$A112/m$ (12)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$

(*Continued on the preceding page*)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 13, pp. 109–111.

C_{2h}^4 $P12/c1$ No. 13 $P2/c$

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
4 g 1	(1) x,y,z (2) $\bar{x},y,\bar{z}+\frac{1}{2}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1c1$ (7)	1; 4		
[2] $P121$ (3)	1; 2		$0,0,1/4$
[2] $P\bar{1}$ (2)	1; 3		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$P12_1/c1$ (14)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P12_1/c1$ (14)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$P12/c1$ (13)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P12/c1$ (13)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a}$			
$P12/c1$ (13)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P12/c1$ (13)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$P12/n1$ (13, $P12/c1$)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	
$P12/n1$ (13, $P12/c1$)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
$C12/c1$ (15)	$\langle 2;\ 3\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$C12/c1$ (15)	$\langle 2;\ 3+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C12/c1$ (15)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C12/c1$ (15)	$\langle 2+(1,0,0);\ 3+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $P12/c1$ (13)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $P12/c1$ (13)	$\langle 2;\ 3+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P12/c1$ (13)	$\langle 2;\ 3+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P12/c1$ (13)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P12/c1$ (13)	$\langle 2+(0,0,3);\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P12/c1$ (13)	$\langle 2+(0,0,5);\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $P12/c1$ (13)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $P12/c1$ (13)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P12/c1$ (13)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{c}'=-2\mathbf{a}+\mathbf{c}$			
{ $P12/c1$ (13)	$\langle 3;\ 2+(-1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	
{ $P12/c1$ (13)	$\langle 2+(1,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	$1,0,0$
{ $P12/c1$ (13)	$\langle 2+(3,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{c}'=-4\mathbf{a}+\mathbf{c}$			
{ $P12/c1$ (13)	$\langle 3;\ 2+(-2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-4\mathbf{a}+\mathbf{c}$	
{ $P12/c1$ (13)	$\langle 2+(0,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-4\mathbf{a}+\mathbf{c}$	$1,0,0$
{ $P12/c1$ (13)	$\langle 2+(2,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-4\mathbf{a}+\mathbf{c}$	$2,0,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$P12/c1$ (13)	$\langle 2;\ 3+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$P12/c1$ (13)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 3+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{c}'=-2q\mathbf{a}+\mathbf{c}$			
$P12/c1$ (13)	$\langle 2+(-q+2u,0,0);\ 3+(2u,0,0)\rangle$ $p>2$; $0\le q<p$; $0\le u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a},\mathbf{b},-2q\mathbf{a}+\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] *Pnnn* (48); [2] *Pccm* (49); [2] *Pban* (50); [2] *Pmma* (51); [2] *Pnna* (52); [2] *Pmna* (53); [2] *Pcca* (54); [2] *Pccn* (56); [2] *Pbcm* (57); [2] *Pmmn* (59); [2] *Pbcn* (60); [2] *Cmme* (67); [2] *Ccce* (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A12/m1$ (12, $C12/m1$); [2] $C12/c1$ (15); [2] $I12/c1$ (15, $C12/c1$)

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P12/m1$ (10)

I Minimal *translationengleiche* supergroups

[2] *Pnnn* (48); [2] *Pccm* (49); [2] *Pban* (50); [2] *Pmma* (51); [2] *Pnna* (52); [2] *Pmna* (53); [2] *Pcca* (54); [2] *Pccn* (56); [2] *Pbcm* (57); [2] *Pmmn* (59); [2] *Pbcn* (60); [2] *Cmme* (67); [2] *Ccce* (68); [2] $P4/n$ (85); [2] $P4_2/n$ (86)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A112/a$ (15); [2] $B112/m$ (12, $A112/m$); [2] $I112/a$ (15, $A112/a$)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $P112/m$ (10)

C_{2h}^4 $\qquad$ $P112/a$ $\qquad$ No. 13 $\qquad$ $P2/c$

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	g	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x+\frac{1}{2},y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P11a$ (7)	1; 4		
[2] $P112$ (3)	1; 2		$1/4,0,0$
[2] $P\bar{1}$ (2)	1; 3		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P112_1/a$ (14)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P112_1/a$ (14)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P112/a$ (13)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P112/a$ (13)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{b}'=2\mathbf{b}$			
$P112/a$ (13)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P112/a$ (13)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$P112/n$ (13, $P112/a$)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a}-2\mathbf{b},2\mathbf{b},\mathbf{c}$	
$P112/n$ (13, $P112/a$)	$\langle 2+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a}-2\mathbf{b},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$A112/a$ (15)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$A112/a$ (15)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$A112/a$ (15)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$A112/a$ (15)	$\langle 2+(0,1,0);\ 3+(0,1,1)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P112/a$ (13)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P112/a$ (13)	$\langle 2;\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P112/a$ (13)	$\langle 2;\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P112/a$ (13)	$\langle 3;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112/a$ (13)	$\langle 2+(3,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P112/a$ (13)	$\langle 2+(5,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P112/a$ (13)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$P112/a$ (13)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112/a$ (13)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\ \mathbf{b}'=3\mathbf{b}$			
$P112/a$ (13)	$\langle 3;\ 2+(0,-1,0)\rangle$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	
$P112/a$ (13)	$\langle 2+(0,1,0);\ 3+(0,2,0)\rangle$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112/a$ (13)	$\langle 2+(0,3,0);\ 3+(0,4,0)\rangle$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{b},\ \mathbf{b}'=3\mathbf{b}$			
$P112/a$ (13)	$\langle 3;\ 2+(0,-2,0)\rangle$	$\mathbf{a}-4\mathbf{b},3\mathbf{b},\mathbf{c}$	
$P112/a$ (13)	$\langle 2+(0,0,0);\ 3+(0,2,0)\rangle$	$\mathbf{a}-4\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112/a$ (13)	$\langle 2+(0,2,0);\ 3+(0,4,0)\rangle$	$\mathbf{a}-4\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,2,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P112/a$ (13)	$\langle 2;\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$			
$P112/a$ (13)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 3+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{a}'=\mathbf{a}-2q\mathbf{b},\ \mathbf{b}'=p\mathbf{b}$			
$P112/a$ (13)	$\langle 2+(0,-q+2u,0);\ 3+(0,2u,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-2q\mathbf{b},p\mathbf{b},\mathbf{c}$	$0,u,0$

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$P2_1/c$ No. 14 $P12_1/c1$ C_{2h}^5

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
4 e 1	(1) x,y,z (2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1c1$ (7)	1; 4	$0,1/4,0$
[2] $P12_11$ (4)	1; 2	$0,0,1/4$
[2] $P\bar{1}$ (2)	1; 3	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$P12_1/c1$ (14)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P12_1/c1$ (14)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$P12_1/n1$ (14, $P12_1/c1$)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	
$P12_1/n1$ (14, $P12_1/c1$)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P12_1/c1$ (14)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$P12_1/c1$ (14)	$\langle 2+(0,1,0);\ 3+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P12_1/c1$ (14)	$\langle 2+(0,1,0);\ 3+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P12_1/c1$ (14)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P12_1/c1$ (14)	$\langle 2+(0,0,3);\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P12_1/c1$ (14)	$\langle 2+(0,0,5);\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P12_1/c1$ (14)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P12_1/c1$ (14)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P12_1/c1$ (14)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{c}'=-2\mathbf{a}+\mathbf{c}$			
$P12_1/c1$ (14)	$\langle 3;\ 2+(-1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	
$P12_1/c1$ (14)	$\langle 2+(1,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	$1,0,0$
$P12_1/c1$ (14)	$\langle 2+(3,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{c}'=-4\mathbf{a}+\mathbf{c}$			
$P12_1/c1$ (14)	$\langle 3;\ 2+(-2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-4\mathbf{a}+\mathbf{c}$	
$P12_1/c1$ (14)	$\langle 2+(0,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-4\mathbf{a}+\mathbf{c}$	$1,0,0$
$P12_1/c1$ (14)	$\langle 2+(2,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},-4\mathbf{a}+\mathbf{c}$	$2,0,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$P12_1/c1$ (14)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2},0);\ 3+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$P12_1/c1$ (14)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a},\ \mathbf{c}'=-2q\mathbf{a}+\mathbf{c}$			
$P12_1/c1$ (14)	$\langle 2+(-q+2u,0,0);\ 3+(2u,0,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a},\mathbf{b},-2q\mathbf{a}+\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] *Pnna* (52); [2] *Pmna* (53); [2] *Pcca* (54); [2] *Pbam* (55); [2] *Pccn* (56); [2] *Pbcm* (57); [2] *Pnnm* (58); [2] *Pbcn* (60); [2] *Pbca* (61); [2] *Pnma* (62); [2] *Cmce* (64)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A12/m1$ (12, $C12/m1$); [2] $C12/c1$ (15); [2] $I12/c1$ (15, $C12/c1$)

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P12_1/m1$ (11); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P12/c1$ (13)

(*Continued from the following page*)

I Minimal *translationengleiche* supergroups

[2] *Pnna* (52); [2] *Pmna* (53); [2] *Pcca* (54); [2] *Pbam* (55); [2] *Pccn* (56); [2] *Pbcm* (57); [2] *Pnnm* (58); [2] *Pbcn* (60); [2] *Pbca* (61); [2] *Pnma* (62); [2] *Cmce* (64)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A112/a$ (15); [2] $B112/m$ (12, $A112/m$); [2] $I112/a$ (15, $A112/a$)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $P112_1/m$ (11); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112/a$ (13)

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	e	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P11a$ (7)	1; 4	$0,0,1/4$
[2] $P112_1$ (4)	1; 2	$1/4,0,0$
[2] $P\bar{1}$ (2)	1; 3	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$P112_1/a$ (14)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P112_1/a$ (14)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$P112_1/n$ (14, $P112_1/a$)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a}-2\mathbf{b},2\mathbf{b},\mathbf{c}$	
$P112_1/n$ (14, $P112_1/a$)	$\langle 2+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a}-2\mathbf{b},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P112_1/a$ (14)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P112_1/a$ (14)	$\langle 2+(0,0,1);\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P112_1/a$ (14)	$\langle 2+(0,0,1);\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P112_1/a$ (14)	$\langle 3;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P112_1/a$ (14)	$\langle 2+(3,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P112_1/a$ (14)	$\langle 2+(5,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P112_1/a$ (14)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$P112_1/a$ (14)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112_1/a$ (14)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{b},\ \mathbf{b}'=3\mathbf{b}$			
$P112_1/a$ (14)	$\langle 3;\ 2+(0,-1,0)\rangle$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	
$P112_1/a$ (14)	$\langle 2+(0,1,0);\ 3+(0,2,0)\rangle$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112_1/a$ (14)	$\langle 2+(0,3,0);\ 3+(0,4,0)\rangle$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{b},\ \mathbf{b}'=3\mathbf{b}$			
$P112_1/a$ (14)	$\langle 3;\ 2+(0,-2,0)\rangle$	$\mathbf{a}-4\mathbf{b},3\mathbf{b},\mathbf{c}$	
$P112_1/a$ (14)	$\langle 2+(0,0,0);\ 3+(0,2,0)\rangle$	$\mathbf{a}-4\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P112_1/a$ (14)	$\langle 2+(0,2,0);\ 3+(0,4,0)\rangle$	$\mathbf{a}-4\mathbf{b},3\mathbf{b},\mathbf{c}$	$0,2,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P112_1/a$ (14)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$			
$P112_1/a$ (14)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 3+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{a}'=\mathbf{a}-2q\mathbf{b},\ \mathbf{b}'=p\mathbf{b}$			
$P112_1/a$ (14)	$\langle 2+(0,-q+2u,0);\ 3+(0,2u,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-2q\mathbf{b},p\mathbf{b},\mathbf{c}$	$0,u,0$

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International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 15, pp. 115–117.

C_{2h}^6 $C\,1\,2/c\,1$ No. 15 $C\,2/c$

UNIQUE AXIS b, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$
8	f	1	(1) x,y,z (2) $\bar{x},y,\bar{z}+\frac{1}{2}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $C1c1$ (9)	(1; 4)+		
[2] $C121$ (5)	(1; 2)+		$0,0,1/4$
[2] $C\bar{1}$ (2, $P\bar{1}$)	(1; 3)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P12_1/n1$ (14, $P12_1/c1$)	1; 3; $(2;\,4)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2] $P12_1/c1$ (14)	1; 4; $(2;\,3)+(\frac{1}{2},\frac{1}{2},0)$		$1/4,1/4,0$
[2] $P12/c1$ (13)	1; 2; 3; 4		
[2] $P12/n1$ (13, $P12/c1$)	1; 2; $(3;\,4)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	$1/4,1/4,0$

- **Enlarged unit cell**

[3] $\mathbf{b}'=3\mathbf{b}$			
$C12/c1$ (15)	$\langle 2;\,3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$C12/c1$ (15)	$\langle 2;\,3+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$C12/c1$ (15)	$\langle 2;\,3+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$C12/c1$ (15)	$\langle 3;\,2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$C12/c1$ (15)	$\langle 2+(0,0,3);\,3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$C12/c1$ (15)	$\langle 2+(0,0,5);\,3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-2\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$C12/c1$ (15)	$\langle 3;\,2+(0,0,1)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	
$C12/c1$ (15)	$\langle 2+(0,0,3);\,3+(0,0,2)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
$C12/c1$ (15)	$\langle 2+(0,0,5);\,3+(0,0,4)\rangle$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=\mathbf{a}-4\mathbf{c}$, $\mathbf{c}'=3\mathbf{c}$			
$C12/c1$ (15)	$\langle 3;\,2+(0,0,1)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	
$C12/c1$ (15)	$\langle 2+(0,0,3);\,3+(0,0,2)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,1$
$C12/c1$ (15)	$\langle 2+(0,0,5);\,3+(0,0,4)\rangle$	$\mathbf{a}-4\mathbf{c},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$C12/c1$ (15)	$\langle 2;\,3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$C12/c1$ (15)	$\langle (2;\,3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$C12/c1$ (15)	$\langle (2;\,3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{b}'=p\mathbf{b}$			
$C12/c1$ (15)	$\langle 2;\,3+(0,2u,0)\rangle$ $p>2$; $0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{a}'=\mathbf{a}-2q\mathbf{c}$, $\mathbf{c}'=p\mathbf{c}$			
$C12/c1$ (15)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\,3+(0,0,2u)\rangle$ $p>2$; $0\leq q<p$; $0\leq u<p$ p conjugate subgroups for each pair of q and prime p	$\mathbf{a}-2q\mathbf{c},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p] $\mathbf{a}'=p\mathbf{a}$			
$C12/c1$ (15)	$\langle (2;\,3)+(2u,0,0)\rangle$ $p>2$; $0\leq u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] *Cmcm* (63); [2] *Cmce* (64); [2] *Cccm* (66); [2] *Ccce* (68); [2] *Fddd* (70); [2] *Ibam* (72); [2] *Ibca* (73); [2] *Imma* (74); [2] $I4_1/a$ (88); [3] $P\bar{3}12/c$ (163, $P\bar{3}1c$); [3] $P\bar{3}2/c1$ (165, $P\bar{3}c1$); [3] $R\bar{3}2/c$ (167, $R\bar{3}c$)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $F12/m1$ (12, $C12/m1$)

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C12/m1$ (12); [2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P12/c1$ (13)

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I Minimal *translationengleiche* supergroups

[2] *Cmcm* (63); [2] *Cmce* (64); [2] *Cccm* (66); [2] *Ccce* (68); [2] *Fddd* (70); [2] *Ibam* (72); [2] *Ibca* (73); [2] *Imma* (74); [2] $I4_1/a$ (88); [3] $P\bar{3}12/c$ (163, $P\bar{3}1c$); [3] $P\bar{3}2/c1$ (165, $P\bar{3}c1$); [3] $R\bar{3}2/c$ (167, $R\bar{3}c$)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $F112/m$ (12, $A112/m$)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $A112/m$ (12); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P112/a$ (13)

UNIQUE AXIS c, CELL CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$
8	f	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x+\frac{1}{2},y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $A11a$ (9)	(1; 4)+		
[2] $A112$ (5)	(1; 2)+		$1/4,0,0$
[2] $A\bar{1}$ (2, $P\bar{1}$)	(1; 3)+	$\mathbf{a},1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P112_1/n$ (14, $P112_1/a$)	1; 3; $(2;\ 4)+(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P112_1/a$ (14)	1; 4; $(2;\ 3)+(0,\frac{1}{2},\frac{1}{2})$		$0,1/4,1/4$
[2] $P112/a$ (13)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; $(3;\ 4)+(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/4,1/4$

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$A112/a$ (15)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$A112/a$ (15)	$\langle 2;\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$A112/a$ (15)	$\langle 2;\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$A112/a$ (15)	$\langle 3;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$A112/a$ (15)	$\langle 2+(3,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$A112/a$ (15)	$\langle 2+(5,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-2\mathbf{a}+\mathbf{b}$			
$A112/a$ (15)	$\langle 3;\ 2+(1,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	
$A112/a$ (15)	$\langle 2+(3,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$A112/a$ (15)	$\langle 2+(5,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=-4\mathbf{a}+\mathbf{b}$			
$A112/a$ (15)	$\langle 3;\ 2+(1,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	
$A112/a$ (15)	$\langle 2+(3,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	$1,0,0$
$A112/a$ (15)	$\langle 2+(5,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},-4\mathbf{a}+\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$A112/a$ (15)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$A112/a$ (15)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$A112/a$ (15)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$A112/a$ (15)	$\langle 2;\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=-2q\mathbf{a}+\mathbf{b}$			
$A112/a$ (15)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 3+(2u,0,0)\rangle$ $p>2;\ 0\le q<p;\ 0\le u<p$ p conjugate subgroups for each pair of q and prime p	$p\mathbf{a},-2q\mathbf{a}+\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$A112/a$ (15)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$

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$P222$ No. 16 $P222$ D_2^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	u	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P112$ (3)	1; 2		
[2] $P121$ (3)	1; 3		
[2] $P211$ (3, $P121$)	1; 4	**c**, **a**, **b**	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$			
$P2_122$ (17, $P222_1$)	$\langle 3;\ 2+(1,0,0)\rangle$	**b**, **c**, 2**a**	
$P2_122$ (17, $P222_1$)	$\langle 2;\ 3+(1,0,0)\rangle$	**b**, **c**, 2**a**	1/2, 0, 0
$P222$ (16)	$\langle 2;\ 3\rangle$	2**a**, **b**, **c**	
$P222$ (16)	$\langle (2;\ 3)+(1,0,0)\rangle$	2**a**, **b**, **c**	1/2, 0, 0
[2] $\mathbf{b}' = 2\mathbf{b}$			
$P22_12$ (17, $P222_1$)	$\langle 2;\ 3+(0,1,0)\rangle$	**c**, **a**, 2**b**	
$P22_12$ (17, $P222_1$)	$\langle (2;\ 3)+(0,1,0)\rangle$	**c**, **a**, 2**b**	0, 1/2, 0
$P222$ (16)	$\langle 2;\ 3\rangle$	**a**, 2**b**, **c**	
$P222$ (16)	$\langle 3;\ 2+(0,1,0)\rangle$	**a**, 2**b**, **c**	0, 1/2, 0
[2] $\mathbf{c}' = 2\mathbf{c}$			
$P222_1$ (17)	$\langle 3;\ 2+(0,0,1)\rangle$	**a**, **b**, 2**c**	0, 0, 1/2
$P222_1$ (17)	$\langle (2;\ 3)+(0,0,1)\rangle$	**a**, **b**, 2**c**	
$P222$ (16)	$\langle 2;\ 3\rangle$	**a**, **b**, 2**c**	
$P222$ (16)	$\langle 2;\ 3+(0,0,1)\rangle$	**a**, **b**, 2**c**	0, 0, 1/2
[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$A222$ (21, $C222$)	$\langle 2;\ 3\rangle$	2**b**, 2**c**, **a**	
$A222$ (21, $C222$)	$\langle 3;\ 2+(0,1,0)\rangle$	2**b**, 2**c**, **a**	0, 1/2, 0
$A222$ (21, $C222$)	$\langle 2;\ 3+(0,0,1)\rangle$	2**b**, 2**c**, **a**	0, 0, 1/2
$A222$ (21, $C222$)	$\langle 2+(0,1,0);\ 3+(0,0,1)\rangle$	2**b**, 2**c**, **a**	0, 1/2, 1/2
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$			
$B222$ (21, $C222$)	$\langle 2;\ 3\rangle$	2**c**, 2**a**, **b**	
$B222$ (21, $C222$)	$\langle 2;\ 3+(0,0,1)\rangle$	2**c**, 2**a**, **b**	0, 0, 1/2
$B222$ (21, $C222$)	$\langle (2;\ 3)+(1,0,0)\rangle$	2**c**, 2**a**, **b**	1/2, 0, 0
$B222$ (21, $C222$)	$\langle 2+(1,0,0);\ 3+(1,0,1)\rangle$	2**c**, 2**a**, **b**	1/2, 0, 1/2
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$			
$C222$ (21)	$\langle 2;\ 3\rangle$	2**a**, 2**b**, **c**	
$C222$ (21)	$\langle (2;\ 3)+(1,0,0)\rangle$	2**a**, 2**b**, **c**	1/2, 0, 0
$C222$ (21)	$\langle 3;\ 2+(0,1,0)\rangle$	2**a**, 2**b**, **c**	0, 1/2, 0
$C222$ (21)	$\langle 2+(1,1,0);\ 3+(1,0,0)\rangle$	2**a**, 2**b**, **c**	1/2, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
$F222$ (22)	$\langle 2;\ 3\rangle$	2**a**, 2**b**, 2**c**	
$F222$ (22)	$\langle 3;\ 2+(0,1,0)\rangle$	2**a**, 2**b**, 2**c**	0, 1/2, 0
$F222$ (22)	$\langle 2;\ 3+(0,0,1)\rangle$	2**a**, 2**b**, 2**c**	0, 0, 1/2
$F222$ (22)	$\langle (2;\ 3)+(1,0,0)\rangle$	2**a**, 2**b**, 2**c**	1/2, 0, 0
[3] $\mathbf{a}' = 3\mathbf{a}$			
$P222$ (16)	$\langle 2;\ 3\rangle$	3**a**, **b**, **c**	
$P222$ (16)	$\langle (2;\ 3)+(2,0,0)\rangle$	3**a**, **b**, **c**	1, 0, 0
$P222$ (16)	$\langle (2;\ 3)+(4,0,0)\rangle$	3**a**, **b**, **c**	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$P222$ (16)	$\langle 2;\ 3\rangle$	**a**, 3**b**, **c**	
$P222$ (16)	$\langle 3;\ 2+(0,2,0)\rangle$	**a**, 3**b**, **c**	0, 1, 0
$P222$ (16)	$\langle 3;\ 2+(0,4,0)\rangle$	**a**, 3**b**, **c**	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P222$ (16)	$\langle 2;\ 3\rangle$	**a**, **b**, 3**c**	
$P222$ (16)	$\langle 2;\ 3+(0,0,2)\rangle$	**a**, **b**, 3**c**	0, 0, 1
$P222$ (16)	$\langle 2;\ 3+(0,0,4)\rangle$	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
$P222$ (16)	$\langle(2;\ 3) + (2u,0,0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
$P222$ (16)	$\langle 3;\ 2 + (0,2u,0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$P222$ (16)	$\langle 2;\ 3 + (0,0,2u)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] *Pmmm* (47); [2] *Pnnn* (48); [2] *Pccm* (49); [2] *Pban* (50); [2] *P*422 (89); [2] $P4_222$ (93); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2m$ (111); [3] *P*23 (195)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *A*222 (21, *C*222); [2] *B*222 (21, *C*222); [2] *C*222 (21); [2] *I*222 (23)

- **Decreased unit cell** none

$P222_1$ No. 17 $P222_1$ D_2^2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	e	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x,\bar{y},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P112_1$ (4)	1; 2		
[2] $P121$ (3)	1; 3		$0,0,1/4$
[2] $P211$ (3, $P121$)	1; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$P2_122_1$ (18, $P2_12_12$)	$\langle 2;\ 3+(1,0,0)\rangle$	$\mathbf{c},2\mathbf{a},\mathbf{b}$	$1/2,0,1/4$
$P2_122_1$ (18, $P2_12_12$)	$\langle 3;\ 2+(1,0,0)\rangle$	$\mathbf{c},2\mathbf{a},\mathbf{b}$	$0,0,1/4$
$P222_1$ (17)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$P222_1$ (17)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$P222_12_1$ (18, $P2_12_12$)	$\langle 2;\ 3+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/2,0$
$P222_12_1$ (18, $P2_12_12$)	$\langle (2;\ 3)+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	
$P222_1$ (17)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P222_1$ (17)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C222_1$ (20)	$\langle 2;\ 3\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$C222_1$ (20)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C222_1$ (20)	$\langle 3;\ 2+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C222_1$ (20)	$\langle 2+(1,1,0);\ 3+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
$P222_1$ (17)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P222_1$ (17)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P222_1$ (17)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P222_1$ (17)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$P222_1$ (17)	$\langle 3;\ 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P222_1$ (17)	$\langle 3;\ 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P222_1$ (17)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P222_1$ (17)	$\langle 2+(0,0,1);\ 3+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P222_1$ (17)	$\langle 2+(0,0,1);\ 3+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$P222_1$ (17)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$P222_1$ (17)	$\langle 3;\ 2+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$P222_1$ (17)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] *Pmma* (51); [2] *Pnna* (52); [2] *Pmna* (53); [2] *Pcca* (54); [2] $P4_122$ (91); [2] $P4_322$ (95)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C222_1$ (20); [2] $A222$ (21, $C222$); [2] $B222$ (21, $C222$); [2] $I2_12_12_1$ (24)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P222$ (16)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 18, p. 121.

D_2^3 $P2_12_12$ No. 18 $P2_12_12$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P12_11$ (4)	1; 3		1/4, 0, 0
[2] $P2_111$ (4, $P12_11$)	1; 4	**c**, **a**, **b**	0, 1/4, 0
[2] $P112$ (3)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P2_12_12_1$ (19)	$\langle 3;\ 2+(0,0,1)\rangle$	**a**, **b**, 2**c**	1/4, 0, 1/2
$P2_12_12_1$ (19)	$\langle (2;\ 3)+(0,0,1)\rangle$	**a**, **b**, 2**c**	1/4, 0, 0
$P2_12_12$ (18)	$\langle 2;\ 3\rangle$	**a**, **b**, 2**c**	
$P2_12_12$ (18)	$\langle 2;\ 3+(0,0,1)\rangle$	**a**, **b**, 2**c**	0, 0, 1/2
[3] $\mathbf{a}'=3\mathbf{a}$			
$P2_12_12$ (18)	$\langle 2;\ 3+(1,0,0)\rangle$	3**a**, **b**, **c**	
$P2_12_12$ (18)	$\langle 2+(2,0,0);\ 3+(3,0,0)\rangle$	3**a**, **b**, **c**	1, 0, 0
$P2_12_12$ (18)	$\langle 2+(4,0,0);\ 3+(5,0,0)\rangle$	3**a**, **b**, **c**	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
$P2_12_12$ (18)	$\langle 2;\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	
$P2_12_12$ (18)	$\langle 2+(0,2,0);\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	0, 1, 0
$P2_12_12$ (18)	$\langle 2+(0,4,0);\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$P2_12_12$ (18)	$\langle 2;\ 3\rangle$	**a**, **b**, 3**c**	
$P2_12_12$ (18)	$\langle 2;\ 3+(0,0,2)\rangle$	**a**, **b**, 3**c**	0, 0, 1
$P2_12_12$ (18)	$\langle 2;\ 3+(0,0,4)\rangle$	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$P2_12_12$ (18)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	p**a**, **b**, **c**	u, 0, 0
[p] $\mathbf{b}'=p\mathbf{b}$			
$P2_12_12$ (18)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	**a**, p**b**, **c**	0, u, 0
[p] $\mathbf{c}'=p\mathbf{c}$			
$P2_12_12$ (18)	$\langle 2;\ 3+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	**a**, **b**, p**c**	0, 0, u

I Minimal *translationengleiche* supergroups

[2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pmmn$ (59); [2] $Pbcn$ (60); [2] $P42_12$ (90); [2] $P4_22_12$ (94); [2] $P\bar{4}2_1m$ (113); [2] $P\bar{4}2_1c$ (114)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A2_122$ (20, $C222_1$); [2] $B22_12$ (20, $C222_1$); [2] $C222$ (21); [2] $I222$ (23)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $P22_12$ (17, $P2221$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $P2_122$ (17, $P222_1$)

$P2_12_12_1$ No. 19 $P2_12_12_1$ D_2^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	a	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P112_1$ (4)	1; 2		$1/4,0,0$
[2] $P12_11$ (4)	1; 3		$0,0,1/4$
[2] $P2_111$ (4, $P12_11$)	1; 4	**c**, **a**, **b**	$0,1/4,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$P2_12_12_1$ (19)	$\langle 3;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$P2_12_12_1$ (19)	$\langle 2+(3,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$P2_12_12_1$ (19)	$\langle 2+(5,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$P2_12_12_1$ (19)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$P2_12_12_1$ (19)	$\langle 2+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$P2_12_12_1$ (19)	$\langle 2+(0,4,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P2_12_12_1$ (19)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P2_12_12_1$ (19)	$\langle 2+(0,0,1);\ 3+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P2_12_12_1$ (19)	$\langle 2+(0,0,1);\ 3+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$P2_12_12_1$ (19)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 3+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$P2_12_12_1$ (19)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$P2_12_12_1$ (19)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] *Pbca* (61); [2] *Pnma* (62); [2] $P4_12_12$ (92); [2] $P4_32_12$ (96); [3] $P2_13$ (198)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $A2_122$ (20, $C222_1$); [2] $B22_12$ (20, $C222_1$); [2] $C222_1$ (20); [2] $I2_12_12_1$ (24)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $P22_12_1$ (18, $P2_12_12$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $P2_122_1$ (18, $P2_12_12$); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P2_12_12$ (18)

D_2^5 $C222_1$ No. 20 $C222_1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$
8	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x,\bar{y},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $C121$ (5)	(1; 3)+		0, 0, 1/4
[2] $C211$ (5, $C121$)	(1; 4)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112_1$ (4, $P112_1$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P2_12_12_1$ (19)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$		1/4, 0, 0
[2] $P2_122_1$ (18, $P2_12_12$)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	0, 1/4, 1/4
[2] $P22_12_1$ (18, $P2_12_12$)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	1/4, 0, 0
[2] $P222_1$ (17)	1; 2; 3; 4		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$C222_1$ (20)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$C222_1$ (20)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$C222_1$ (20)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
$C222_1$ (20)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$C222_1$ (20)	$\langle 3;\ 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$C222_1$ (20)	$\langle 3;\ 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$C222_1$ (20)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$C222_1$ (20)	$\langle 2+(0,0,1);\ 3+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$C222_1$ (20)	$\langle 2+(0,0,1);\ 3+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$C222_1$ (20)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	u, 0, 0
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$C222_1$ (20)	$\langle 3;\ 2+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	0, u, 0
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$C222_1$ (20)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	0, 0, u

I Minimal *translationengleiche* supergroups

[2] $Cmcm$ (63); [2] $Cmce$ (64); [2] $P4_122$ (91); [2] $P4_12_12$ (92); [2] $P4_322$ (95); [2] $P4_32_12$ (96); [3] $P6_122$ (178); [3] $P6_522$ (179); [3] $P6_322$ (182)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $F222$ (22)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $P222_1$ (17); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C222$ (21)

$C222$ No. 21 $C222$ D_2^6

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$

8 l 1 (1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $C121$ (5)	(1; 3)+		
[2] $C211$ (5, $C121$)	(1; 4)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112$ (3, $P112$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

• Loss of centring translations

[2] $P2_12_12$ (18)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $P2_122$ (17, $P222_1$)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/4,0$
[2] $P22_12$ (17, $P222_1$)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
[2] $P222$ (16)	1; 2; 3; 4		

• Enlarged unit cell

[2] $\mathbf{c}'=2\mathbf{c}$			
$I2_12_12_1$ (24)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$3/4,0,0$
$I2_12_12_1$ (24)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$3/4,0,1/2$
$I222$ (23)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$I222$ (23)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$C222$ (21)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$C222$ (21)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$C222_1$ (20)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$C222_1$ (20)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
$C222$ (21)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$C222$ (21)	$\langle (2;\ 3)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$C222$ (21)	$\langle (2;\ 3)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$C222$ (21)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$C222$ (21)	$\langle 3;\ 2+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$C222$ (21)	$\langle 3;\ 2+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$C222$ (21)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$C222$ (21)	$\langle 2;\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$C222$ (21)	$\langle 2;\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

• Series of maximal isomorphic subgroups

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$C222$ (21)	$\langle (2;\ 3)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$C222$ (21)	$\langle 3;\ 2+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$C222$ (21)	$\langle 2;\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $Cmmm$ (65); [2] $Cccm$ (66); [2] $Cmme$ (67); [2] $Ccce$ (68); [2] $P422$ (89); [2] $P42_12$ (90); [2] $P4_222$ (93); [2] $P4_22_12$ (94); [2] $P\bar{4}m2$ (115); [2] $P\bar{4}c2$ (116); [2] $P\bar{4}b2$ (117); [2] $P\bar{4}n2$ (118); [3] $P622$ (177); [3] $P6_222$ (180); [3] $P6_422$ (181)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $F222$ (22)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $P222$ (16)

(*Continued from the following page*)

- **Series of maximal isomorphic subgroups**

$[p]\ \mathbf{a}' = p\mathbf{a}$			
$F222$ (22)	$\langle(2;\ 3) + (2u,0,0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]\ \mathbf{b}' = p\mathbf{b}$			
$F222$ (22)	$\langle 3;\ 2 + (0,2u,0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]\ \mathbf{c}' = p\mathbf{c}$			
$F222$ (22)	$\langle 2;\ 3 + (0,0,2u)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $Fmmm$ (69); [2] $Fddd$ (70); [2] $I422$ (97); [2] $I4_122$ (98); [2] $I\bar{4}m2$ (119); [2] $I\bar{4}c2$ (120); [3] $F23$ (196)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P222$ (16)

$F222$ No. 22 $F222$ D_2^7

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$
16 k 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $F112$ (5, $A112$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}),\mathbf{b},\mathbf{c}$	
[2] $F121$ (5, $C121$)	(1; 3)+	$\mathbf{a},\mathbf{b},1/2(-\mathbf{a}+\mathbf{c})$	
[2] $F211$ (5, $C121$)	(1; 4)+	$\mathbf{c},\mathbf{a},1/2(\mathbf{b}-\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $A222$ (21, $C222$)	1; 2; 3; 4; (1; 2; 3; 4) + $(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $A222$ (21, $C222$)	1; 4; (1; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,1/4,1/4$
[2] $B222$ (21, $C222$)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},0,\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $B222$ (21, $C222$)	1; 3; (1; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,1/4$
[2] $C222$ (21)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $C222$ (21)	1; 2; (1; 2) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$		$1/4,1/4,1/4$
[2] $A2_122$ (20, $C222_1$)	1; 2; (1; 2) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,0,1/4$
[2] $A2_122$ (20, $C222_1$)	1; 3; (1; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/4,0$
[2] $B22_12$ (20, $C222_1$)	1; 2; (1; 2) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $B22_12$ (20, $C222_1$)	1; 4; (1; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
[2] $C222_1$ (20)	1; 3; (1; 3) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$		$0,1/4,1/4$
[2] $C222_1$ (20)	1; 4; (1; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$		$1/4,0,0$

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$F222$ (22)	$\langle 2; 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$F222$ (22)	$\langle (2; 3) + (2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$F222$ (22)	$\langle (2; 3) + (4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$F222$ (22)	$\langle 2; 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$F222$ (22)	$\langle 3; 2 + (0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$F222$ (22)	$\langle 3; 2 + (0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$F222$ (22)	$\langle 2; 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$F222$ (22)	$\langle 2; 3 + (0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$F222$ (22)	$\langle 2; 3 + (0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

(*Continued on the preceding page*)

D_2^8 $I222$ No. 23 $I222$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8	k	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $I112$ (5, $A112$)	(1; 2)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[2] $I121$ (5, $C121$)	(1; 3)+	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $I211$ (5, $C121$)	(1; 4)+	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P2_12_12$ (18)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,0,1/4$
[2] $P2_122_1$ (18, $P2_12_12$)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,1/4,0$
[2] $P22_12_1$ (18, $P2_12_12$)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,0,0$
[2] $P222$ (16)	1; 2; 3; 4		

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$			
$I222$ (23)	$\langle 2; 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$I222$ (23)	$\langle (2; 3) + (2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$I222$ (23)	$\langle (2; 3) + (4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
$I222$ (23)	$\langle 2; 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$I222$ (23)	$\langle 3; 2 + (0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$I222$ (23)	$\langle 3; 2 + (0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$I222$ (23)	$\langle 2; 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I222$ (23)	$\langle 2; 3 + (0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I222$ (23)	$\langle 2; 3 + (0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
$I222$ (23)	$\langle (2; 3) + (2u,0,0)\rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
$I222$ (23)	$\langle 3; 2 + (0,2u,0)\rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$I222$ (23)	$\langle 2; 3 + (0,0,2u)\rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $Immm$ (71); [2] $Ibam$ (72); [2] $I422$ (97); [2] $I\bar{4}2m$ (121); [3] $I23$ (197)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $A222$ (21, $C222$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $B222$ (21, $C222$); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C222$ (21)

$I2_12_12_1$ No. 24 $I2_12_12_1$ D_2^9

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8	*d*	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $I112_1$ (5, $A112$)	(1; 2)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,1/4,0$
[2] $I12_11$ (5, $C121$)	(1; 3)+	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	$1/4,0,0$
[2] $I2_111$ (5, $C121$)	(1; 4)+	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P2_12_12_1$ (19)	1; 2; 3; 4		
[2] $P222_1$ (17)	1; 2; $(3;\ 4)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,0,1/4$
[2] $P22_12$ (17, $P222_1$)	1; 3; $(2;\ 4)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,1/4,1/4$
[2] $P2_122$ (17, $P222_1$)	1; 4; $(2;\ 3)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,1/4,0$

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$I2_12_12_1$ (24)	$\langle 3;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$I2_12_12_1$ (24)	$\langle 2+(3,0,0);\ 3+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$I2_12_12_1$ (24)	$\langle 2+(5,0,0);\ 3+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$I2_12_12_1$ (24)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$I2_12_12_1$ (24)	$\langle 2+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$I2_12_12_1$ (24)	$\langle 2+(0,4,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$I2_12_12_1$ (24)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I2_12_12_1$ (24)	$\langle 2+(0,0,1);\ 3+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I2_12_12_1$ (24)	$\langle 2+(0,0,1);\ 3+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$I2_12_12_1$ (24)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 3+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$I2_12_12_1$ (24)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$I2_12_12_1$ (24)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] *Ibca* (73); [2] *Imma* (74); [2] $I4_122$ (98); [2] $I\bar{4}2d$ (122); [3] $I2_13$ (199)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $A222$ (21, $C222$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $B222$ (21, $C222$); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C222$ (21)

C_{2v}^1 $Pmm2$ No. 25 $Pmm2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	i	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $P1m1$ (6)	1; 3		
[2] $Pm11$ (6, $P1m1$)	1; 4	**c**, **a**, **b**	
[2] $P112$ (3)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$			
$Pma2$ (28)	$\langle 2;\ 3+(1,0,0)\rangle$	2**a**, **b**, **c**	
$Pma2$ (28)	$\langle (2;\ 3)+(1,0,0)\rangle$	2**a**, **b**, **c**	1/2, 0, 0
$Pmm2$ (25)	$\langle 2;\ 3\rangle$	2**a**, **b**, **c**	
$Pmm2$ (25)	$\langle 3;\ 2+(1,0,0)\rangle$	2**a**, **b**, **c**	1/2, 0, 0
[2] $\mathbf{b}' = 2\mathbf{b}$			
$Pbm2$ (28, $Pma2$)	$\langle 2;\ 3+(0,1,0)\rangle$	−2**b**, **a**, **c**	
$Pbm2$ (28, $Pma2$)	$\langle 3;\ 2+(0,1,0)\rangle$	−2**b**, **a**, **c**	0, 1/2, 0
$Pmm2$ (25)	$\langle 2;\ 3\rangle$	**a**, 2**b**, **c**	
$Pmm2$ (25)	$\langle (2;\ 3)+(0,1,0)\rangle$	**a**, 2**b**, **c**	0, 1/2, 0
[2] $\mathbf{c}' = 2\mathbf{c}$			
$Pcc2$ (27)	$\langle 2;\ 3+(0,0,1)\rangle$	**a**, **b**, 2**c**	
$Pmc2_1$ (26)	$\langle (2;\ 3)+(0,0,1)\rangle$	**a**, **b**, 2**c**	
$Pcm2_1$ (26, $Pmc2_1$)	$\langle 3;\ 2+(0,0,1)\rangle$	−**b**, **a**, 2**c**	
$Pmm2$ (25)	$\langle 2;\ 3\rangle$	**a**, **b**, 2**c**	
[2] $\mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$Aem2$ (39)	$\langle 2;\ 3+(0,1,0)\rangle$	**a**, 2**b**, 2**c**	
$Aem2$ (39)	$\langle 3;\ 2+(0,1,0)\rangle$	**a**, 2**b**, 2**c**	0, 1/2, 0
$Amm2$ (38)	$\langle 2;\ 3\rangle$	**a**, 2**b**, 2**c**	
$Amm2$ (38)	$\langle (2;\ 3)+(0,1,0)\rangle$	**a**, 2**b**, 2**c**	0, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{c}' = 2\mathbf{c}$			
$Bme2$ (39, $Aem2$)	$\langle 2;\ 3+(1,0,0)\rangle$	−**b**, 2**a**, 2**c**	
$Bme2$ (39, $Aem2$)	$\langle (2;\ 3)+(1,0,0)\rangle$	−**b**, 2**a**, 2**c**	1/2, 0, 0
$Bmm2$ (38, $Amm2$)	$\langle 2;\ 3\rangle$	−**b**, 2**a**, 2**c**	
$Bmm2$ (38, $Amm2$)	$\langle 3;\ 2+(1,0,0)\rangle$	−**b**, 2**a**, 2**c**	1/2, 0, 0
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$Cmm2$ (35)	$\langle 2;\ 3\rangle$	2**a**, 2**b**, **c**	
$Cmm2$ (35)	$\langle 3;\ 2+(1,0,0)\rangle$	2**a**, 2**b**, **c**	1/2, 0, 0
$Cmm2$ (35)	$\langle (2;\ 3)+(0,1,0)\rangle$	2**a**, 2**b**, **c**	0, 1/2, 0
$Cmm2$ (35)	$\langle 2+(1,1,0);\ 3+(0,1,0)\rangle$	2**a**, 2**b**, **c**	1/2, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$Fmm2$ (42)	$\langle 2;\ 3\rangle$	2**a**, 2**b**, 2**c**	
$Fmm2$ (42)	$\langle 3;\ 2+(1,0,0)\rangle$	2**a**, 2**b**, 2**c**	1/2, 0, 0
$Fmm2$ (42)	$\langle (2;\ 3)+(0,1,0)\rangle$	2**a**, 2**b**, 2**c**	0, 1/2, 0
$Fmm2$ (42)	$\langle 2+(1,1,0);\ 3+(0,1,0)\rangle$	2**a**, 2**b**, 2**c**	1/2, 1/2, 0
[3] $\mathbf{a}' = 3\mathbf{a}$			
$Pmm2$ (25)	$\langle 2;\ 3\rangle$	3**a**, **b**, **c**	
$Pmm2$ (25)	$\langle 3;\ 2+(2,0,0)\rangle$	3**a**, **b**, **c**	1, 0, 0
$Pmm2$ (25)	$\langle 3;\ 2+(4,0,0)\rangle$	3**a**, **b**, **c**	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$Pmm2$ (25)	$\langle 2;\ 3\rangle$	**a**, 3**b**, **c**	
$Pmm2$ (25)	$\langle (2;\ 3)+(0,2,0)\rangle$	**a**, 3**b**, **c**	0, 1, 0
$Pmm2$ (25)	$\langle (2;\ 3)+(0,4,0)\rangle$	**a**, 3**b**, **c**	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$Pmm2$ (25)	$\langle 2;\ 3\rangle$	**a**, **b**, 3**c**	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
*Pmm*2 (25)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
*Pmm*2 (25)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
*Pmm*2 (25)	$\langle 2;\ 3\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] *Pmmm* (47); [2] *Pmma* (51); [2] *Pmmn* (59); [2] *P*4*mm* (99); [2] $P4_2mc$ (105); [2] $P\bar{4}m2$ (115)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Cmm*2 (35); [2] *Amm*2 (38); [2] *Bmm*2 (38, *Amm*2); [2] *Imm*2 (44)

- **Decreased unit cell** none

C_{2v}^{2} $Pmc2_1$ No. 26 $Pmc2_1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $x,\bar{y},z+\frac{1}{2}$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $P1c1$ (7)	1; 3		
[2] $Pm11$ (6, $P1m1$)	1; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $P112_1$ (4)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$Pmn2_1$ (31)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Pmn2_1$ (31)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pmc2_1$ (26)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pmc2_1$ (26)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$Pbc2_1$ (29, $Pca2_1$)	$\langle 2;\ 3+(0,1,0)\rangle$	$-2\mathbf{b},\mathbf{a},\mathbf{c}$	
$Pbc2_1$ (29, $Pca2_1$)	$\langle 3;\ 2+(0,1,0)\rangle$	$-2\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/2,0$
$Pmc2_1$ (26)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pmc2_1$ (26)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$Cmc2_1$ (36)	$\langle 2;\ 3\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Cmc2_1$ (36)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Cmc2_1$ (36)	$\langle (2;\ 3)+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$Cmc2_1$ (36)	$\langle 2+(1,1,0);\ 3+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Pmc2_1$ (26)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Pmc2_1$ (26)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Pmc2_1$ (26)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Pmc2_1$ (26)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Pmc2_1$ (26)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Pmc2_1$ (26)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pmc2_1$ (26)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pmc2_1$ (26)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pmc2_1$ (26)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pmc2_1$ (26)	$\langle (2;\ 3)+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] *Pmma* (51); [2] *Pbam* (55); [2] *Pbcm* (57); [2] *Pnma* (62)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmc2_1$ (36); [2] *Amm*2 (38); [2] *Bme*2 (39, *Aem*2); [2] *Ima*2 (46)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ *Pmm*2 (25)

$Pcc2$ No. 27 $Pcc2$ C_{2v}^{3}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	e	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z+\frac{1}{2}$ (4) $\bar{x},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1c1$ (7)	1; 3		
[2] $Pc11$ (7, $P1c1$)	1; 4	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P112$ (3)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$Pcn2$ (30, $Pnc2$)	$\langle 2;\ 3+(1,0,0)\rangle$	$-\mathbf{b},2\mathbf{a},\mathbf{c}$	
$Pcn2$ (30, $Pnc2$)	$\langle (2;\ 3)+(1,0,0)\rangle$	$-\mathbf{b},2\mathbf{a},\mathbf{c}$	$1/2,0,0$
$Pcc2$ (27)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pcc2$ (27)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$Pnc2$ (30)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pnc2$ (30)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$Pcc2$ (27)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pcc2$ (27)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$Ccc2$ (37)	$\langle 2;\ 3\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Ccc2$ (37)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Ccc2$ (37)	$\langle (2;\ 3)+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$Ccc2$ (37)	$\langle 2+(1,1,0);\ 3+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Pcc2$ (27)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Pcc2$ (27)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Pcc2$ (27)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Pcc2$ (27)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Pcc2$ (27)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Pcc2$ (27)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pcc2$ (27)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pcc2$ (27)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pcc2$ (27)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pcc2$ (27)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Pccm$ (49); [2] $Pcca$ (54); [2] $Pccn$ (56); [2] $P4_2cm$ (101); [2] $P4cc$ (103); [2] $P\bar{4}c2$ (116)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Ccc2$ (37); [2] $Aem2$ (39); [2] $Bme2$ (39, $Aem2$); [2] $Iba2$ (45)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pmm2$ (25)

C_{2v}^4 $Pma2$ No. 28 $Pma2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	d	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y},z$ (4) $\bar{x}+\frac{1}{2},y,z$

I Maximal *translationengleiche* subgroups

[2] $P1a1$ (7, $P1c1$)	1; 3	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $Pm11$ (6, $P1m1$)	1; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,0,0$
[2] $P112$ (3)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$Pba2$ (32)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pba2$ (32)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$Pma2$ (28)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pma2$ (28)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{c}'=2\mathbf{c}$			
$Pmn2_1$ (31)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$1/4,0,0$
$Pcn2$ (30, $Pnc2$)	$\langle 2;\ 3+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a},2\mathbf{c}$	
$Pca2_1$ (29)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pma2$ (28)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{b}'=2\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$Aea2$ (41)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Aea2$ (41)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$Ama2$ (40)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Ama2$ (40)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Pma2$ (28)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Pma2$ (28)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Pma2$ (28)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Pma2$ (28)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Pma2$ (28)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Pma2$ (28)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pma2$ (28)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pma2$ (28)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pma2$ (28)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pma2$ (28)	$\langle 2;\ 3\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Pccm$ (49); [2] $Pmma$ (51); [2] $Pmna$ (53); [2] $Pbcm$ (57)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmm2$ (35); [2] $Bme2$ (39, $Aem2$); [2] $Ama2$ (40); [2] $Ima2$ (46)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pmm2$ (25)

$Pca2_1$ No. 29 $Pca2_1$ C_{2v}^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	a	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $x+\frac{1}{2},\bar{y},z$ (4) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1a1$ (7, $P1c1$)	1; 3	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $Pc11$ (7, $P1c1$)	1; 4	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 0, 0
[2] $P112_1$ (4)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$Pna2_1$ (33)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pna2_1$ (33)	$\langle 3;\ 2+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	0, 1/2, 0
$Pca2_1$ (29)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pca2_1$ (29)	$\langle (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	0, 1/2, 0
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Pca2_1$ (29)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Pca2_1$ (29)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
{ $Pca2_1$ (29)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Pca2_1$ (29)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Pca2_1$ (29)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
{ $Pca2_1$ (29)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pca2_1$ (29)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pca2_1$ (29)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pca2_1$ (29)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pca2_1$ (29)	$\langle 3;\ 2+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Pcca$ (54); [2] $Pbcm$ (57); [2] $Pbcn$ (60); [2] $Pbca$ (61)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Ccm2_1$ (36, $Cmc2_1$); [2] $Bme2$ (39, $Aem2$); [2] $Aea2$ (41); [2] $Iba2$ (45)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pcm2_1$ (26, $Pmc2_1$)

C_{2v}^{6} $Pnc2$ No. 30 $Pnc2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (4) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1c1$ (7)	1; 3		$0,1/4,0$
[2] $Pn11$ (7, $P1c1$)	1; 4	$\mathbf{b},\mathbf{a},-\mathbf{b}-\mathbf{c}$	
[2] $P112$ (3)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$Pnn2$ (34)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pnn2$ (34)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Pnc2$ (30)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pnc2$ (30)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pnc2$ (30)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pnc2$ (30)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pnc2$ (30)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pnc2$ (30)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pnc2$ (30)	$\langle 2+(0,2,0);\ 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pnc2$ (30)	$\langle 2+(0,4,0);\ 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pnc2$ (30)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Pnc2$ (30)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Pnc2$ (30)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Pnc2$ (30)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] *Pban* (50); [2] *Pnna* (52); [2] *Pmna* (53); [2] *Pbcn* (60)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Ccc*2 (37); [2] *Amm*2 (38); [2] *Bbe*2 (41, *Aea*2); [2] *Ima*2 (46)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ *Pcc*2 (27); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ *Pbm*2 (28, *Pma*2)

$Pmn2_1$ No. 31 $Pmn2_1$ C_{2v}^7

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	b	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $P1n1$ (7, $P1c1$)	1; 3	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2] $Pm11$ (6, $P1m1$)	1; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $P112_1$ (4)	1; 2		$1/4,0,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$Pbn2_1$ (33, $Pna2_1$)	$\langle 2;\ 3+(0,1,0)\rangle$	$-2\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,0,0$
$Pbn2_1$ (33, $Pna2_1$)	$\langle 3;\ 2+(0,1,0)\rangle$	$-2\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/2,0$
$Pmn2_1$ (31)	$\langle 2;\ 3\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pmn2_1$ (31)	$\langle(2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
$\{$ $Pmn2_1$ (31)	$\langle(2;\ 3)+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pmn2_1$ (31)	$\langle 2+(3,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pmn2_1$ (31)	$\langle 2+(5,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$\{$ $Pmn2_1$ (31)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pmn2_1$ (31)	$\langle(2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pmn2_1$ (31)	$\langle(2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pmn2_1$ (31)	$\langle(2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pmn2_1$ (31)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pmn2_1$ (31)	$\langle(2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pmn2_1$ (31)	$\langle(2;\ 3)+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] *Pmna* (53); [2] *Pnnm* (58); [2] *Pmmn* (59); [2] *Pnma* (62)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmc2_1$ (36); [2] $Bmm2$ (38, $Amm2$); [2] $Ama2$ (40); [2] $Imm2$ (44)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pmc2_1$ (26); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pma2$ (28)

C_{2v}^{8} $\quad$ $Pba2$ $\quad$ No. 32 $\quad$ $Pba2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P1a1$ (7, $P1c1$)	1; 3	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	$0,1/4,0$
[2] $Pb11$ (7, $P1c1$)	1; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,0,0$
[2] $P112$ (3)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$Pnn2$ (34)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pna2_1$ (33)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pbn2_1$ (33, $Pna2_1$)	$\langle (2;\ 3)+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a},2\mathbf{c}$	
$Pba2$ (32)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pba2$ (32)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pba2$ (32)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pba2$ (32)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pba2$ (32)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pba2$ (32)	$\langle 2+(0,2,0);\ 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pba2$ (32)	$\langle 2+(0,4,0);\ 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pba2$ (32)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pba2$ (32)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pba2$ (32)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pba2$ (32)	$\langle 2;\ 3\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Pban$ (50); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $P4bm$ (100); [2] $P4_2bc$ (106); [2] $P\bar{4}b2$ (117)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmm2$ (35); [2] $Aea2$ (41); [2] $Bbe2$ (41, $Aea2$); [2] $Iba2$ (45)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pbm2$ (28, $Pma2$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pma2$ (28)

$Pna2_1$ No. 33 $Pna2_1$ C_{2v}^9

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	*a*	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1a1$ (7, $P1c1$)	1; 3	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	0,1/4,0
[2] $Pn11$ (7, $P1c1$)	1; 4	$\mathbf{b},\mathbf{a},-\mathbf{b}-\mathbf{c}$	1/4,0,0
[2] $P112_1$ (4)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Pna2_1$ (33)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pna2_1$ (33)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1,0,0
$Pna2_1$ (33)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2,0,0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pna2_1$ (33)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pna2_1$ (33)	$\langle 2+(0,2,0);\ 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0,1,0
$Pna2_1$ (33)	$\langle 2+(0,4,0);\ 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0,2,0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pna2_1$ (33)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pna2_1$ (33)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	u,0,0
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pna2_1$ (33)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	0,u,0
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pna2_1$ (33)	$\langle 3;\ 2+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] *Pnna* (52); [2] *Pccn* (56); [2] *Pbcn* (60); [2] *Pnma* (62)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Ccm2_1$ (36, $Cmc2_1$); [2] *Ama*2 (40); [2] *Bbe*2 (41, *Aea*2); [2] *Ima*2 (46)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pca2_1$ (29); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pnm2_1$ (31, $Pmn2_1$); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ *Pba*2 (32)

C_{2v}^{10} $Pnn2$ No. 34 $Pnn2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P1n1$ (7, $P1c1$)	1; 3	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	$0,1/4,0$
[2] $Pn11$ (7, $P1c1$)	1; 4	$\mathbf{b},\mathbf{a},-\mathbf{b}-\mathbf{c}$	$1/4,0,0$
[2] $P112$ (3)	1; 2		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$Fdd2$ (43)	$\langle 2;\ 3\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fdd2$ (43)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,0,0$
$Fdd2$ (43)	$\langle (2;\ 3)+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$Fdd2$ (43)	$\langle 2+(1,1,0);\ 3+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Pnn2$ (34)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Pnn2$ (34)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Pnn2$ (34)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Pnn2$ (34)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Pnn2$ (34)	$\langle 2+(0,2,0);\ 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Pnn2$ (34)	$\langle 2+(0,4,0);\ 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pnn2$ (34)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pnn2$ (34)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pnn2$ (34)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pnn2$ (34)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Pnnn$ (48); [2] $Pnna$ (52); [2] $Pnnm$ (58); [2] $P4_2nm$ (102); [2] $P4nc$ (104); [2] $P\bar{4}n2$ (118)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Ccc2$ (37); [2] $Ama2$ (40); [2] $Bbm2$ (40, $Ama2$); [2] $Imm2$ (44)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pnc2$ (30); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pcn2$ (30, $Pnc2$); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pba2$ (32)

$Cmm2$ No. 35 $Cmm2$ C_{2v}^{11}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},0)+$
8	f	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $C1m1$ (8)	(1; 3)+		
[2] $Cm11$ (8, $C1m1$)	(1; 4)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112$ (3, $P112$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pba2$ (32)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $Pbm2$ (28, $Pma2$)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $Pma2$ (28)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$		$1/4,1/4,0$
[2] $Pmm2$ (25)	1; 2; 3; 4		

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$Ima2$ (46)	$\langle(2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$1/4,1/4,0$
$Ibm2$ (46, $Ima2$)	$\langle 3;\ 2+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a},2\mathbf{c}$	$1/4,1/4,0$
$Iba2$ (45)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Imm2$ (44)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Ccc2$ (37)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Cmc2_1$ (36)	$\langle(2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Ccm2_1$ (36, $Cmc2_1$)	$\langle 3;\ 2+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a},2\mathbf{c}$	
$Cmm2$ (35)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Cmm2$ (35)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Cmm2$ (35)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Cmm2$ (35)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Cmm2$ (35)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Cmm2$ (35)	$\langle(2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Cmm2$ (35)	$\langle(2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Cmm2$ (35)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Cmm2$ (35)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Cmm2$ (35)	$\langle(2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Cmm2$ (35)	$\langle 2;\ 3\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Cmmm$ (65); [2] $Cmme$ (67); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4_2cm$ (101); [2] $P4_2nm$ (102); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2_1m$ (113); [3] $P6mm$ (183)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmm2$ (42)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pmm2$ (25)

C_{2v}^{12} $Cmc2_1$ No. 36 $Cmc2_1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$
8	b	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $x,\bar{y},z+\frac{1}{2}$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $C1c1$ (9)	$(1;\ 3)+$		
[2] $Cm11$ (8, $C1m1$)	$(1;\ 4)+$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112_1$ (4, $P112_1$)	$(1;\ 2)+$	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pbn2_1$ (33, $Pna2_1$)	$1;\ 2;\ (3;\ 4)+(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Pmn2_1$ (31)	$1;\ 4;\ (2;\ 3)+(\frac{1}{2},\frac{1}{2},0)$		$0,1/4,0$
[2] $Pbc2_1$ (29, $Pca2_1$)	$1;\ 3;\ (2;\ 4)+(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $Pmc2_1$ (26)	$1;\ 2;\ 3;\ 4$		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Cmc2_1$ (36)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Cmc2_1$ (36)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Cmc2_1$ (36)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Cmc2_1$ (36)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Cmc2_1$ (36)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Cmc2_1$ (36)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Cmc2_1$ (36)	$\langle (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Cmc2_1$ (36)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Cmc2_1$ (36)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Cmc2_1$ (36)	$\langle (2;\ 3)+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Cmcm$ (63); [2] $Cmce$ (64); [3] $P6_3cm$ (185); [3] $P6_3mc$ (186)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmm2$ (42)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pmc2_1$ (26); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Cmm2$ (35)

$Ccc2$ No. 37 $Ccc2$ C_{2v}^{13}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$
8	d	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z+\frac{1}{2}$ (4) $\bar{x},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $C1c1$ (9)	(1; 3)+		
[2] $Cc11$ (9, $C1c1$)	(1; 4)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112$ (3, $P112$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pnn2$ (34)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $Pnc2$ (30)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$		$1/4,1/4,0$
[2] $Pcn2$ (30, $Pnc2$)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $Pcc2$ (27)	1; 2; 3; 4		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Ccc2$ (37)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Ccc2$ (37)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Ccc2$ (37)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Ccc2$ (37)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Ccc2$ (37)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Ccc2$ (37)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Ccc2$ (37)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Ccc2$ (37)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Ccc2$ (37)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Ccc2$ (37)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Cccm$ (66); [2] $Ccce$ (68); [2] $P4cc$ (103); [2] $P4nc$ (104); [2] $P4_2mc$ (105); [2] $P4_2bc$ (106); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2_1c$ (114); [3] $P6cc$ (184)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmm2$ (42)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pcc2$ (27); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Cmm2$ (35)

C_{2v}^{14} $Amm2$ No. 38 $Amm2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+$
8	f	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $A1m1$ (8, $C1m1$)	(1; 3)+	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2] $Am11$ (6, $P1m1$)	(1; 4)+	$1/2(\mathbf{b}+\mathbf{c}),\mathbf{a},1/2(\mathbf{b}-\mathbf{c})$	
[2] $A112$ (5)	(1; 2)+		

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pnm2_1$ (31, $Pmn2_1$)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Pnc2$ (30)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$		
[2] $Pmc2_1$ (26)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$		$0,1/4,0$
[2] $Pmm2$ (25)	1; 2; 3; 4		

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$Ima2$ (46)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Ima2$ (46)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Imm2$ (44)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Imm2$ (44)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Ama2$ (40)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Ama2$ (40)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Amm2$ (38)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Amm2$ (38)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
$Amm2$ (38)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Amm2$ (38)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Amm2$ (38)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Amm2$ (38)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Amm2$ (38)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Amm2$ (38)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Amm2$ (38)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Amm2$ (38)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Amm2$ (38)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Amm2$ (38)	$\langle 2;\ 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Cmcm$ (63); [2] $Cmmm$ (65); [3] $P\bar{6}m2$ (187); [3] $P\bar{6}2m$ (189)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmm2$ (42)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pmm2$ (25)

$Aem2$ No. 39 $Aem2$ C_{2v}^{15}

Former space-group symbol $Abm2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$
8	d	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y}+\frac{1}{2},z$ (4) $\bar{x},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $A1m1$ (8, $C1m1$)	(1; 3)+	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	$0,1/4,0$
[2] $Ae11$ (7, $P1c1$)	(1; 4)+	$1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a},\mathbf{b}$	
[2] $A112$ (5)	(1; 2)+		

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pbc2_1$ (29, $Pca2_1$)	1; 4; $(2;\ 3)+(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/4,0$
[2] $Pbm2$ (28, $Pma2$)	1; 2; 3; 4	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Pcc2$ (27)	1; 2; $(3;\ 4)+(0,\frac{1}{2},\frac{1}{2})$		
[2] $Pcm2_1$ (26, $Pmc2_1$)	1; 3; $(2;\ 4)+(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/4,0$

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$Ibm2$ (46, $Ima2$)	$\langle 2;\ 3\rangle$	$-\mathbf{b},2\mathbf{a},\mathbf{c}$	
$Ibm2$ (46, $Ima2$)	$\langle 3;\ 2+(1,0,0)\rangle$	$-\mathbf{b},2\mathbf{a},\mathbf{c}$	$1/2,0,0$
$Iba2$ (45)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Iba2$ (45)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Aea2$ (41)	$\langle 2;\ 3+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Aea2$ (41)	$\langle (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Aem2$ (39)	$\langle 2;\ 3\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Aem2$ (39)	$\langle 3;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Aem2$ (39)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Aem2$ (39)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Aem2$ (39)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Aem2$ (39)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Aem2$ (39)	$\langle 2+(0,2,0);\ 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Aem2$ (39)	$\langle 2+(0,4,0);\ 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Aem2$ (39)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Aem2$ (39)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Aem2$ (39)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Aem2$ (39)	$\langle 2;\ 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Cmce$ (64); [2] $Cmme$ (67)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmm2$ (42)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pmm2$ (25)

C_{2v}^{16} *Ama*2 No. 40 *Ama*2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$
8	*c*	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y},z$ (4) $\bar{x}+\frac{1}{2},y,z$

I Maximal *translationengleiche* subgroups

[2] $A1a1$ (9, $C1c1$)	(1; 3)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] $Am11$ (6, $P1m1$)	(1; 4)+	$1/2(\mathbf{b}+\mathbf{c}),\mathbf{a},1/2(\mathbf{b}-\mathbf{c})$	1/4, 0, 0
[2] $A112$ (5)	(1; 2)+		

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pnn2$ (34)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$		
[2] $Pna2_1$ (33)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$		0, 1/4, 0
[2] $Pmn2_1$ (31)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 0
[2] $Pma2$ (28)	1; 2; 3; 4		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Ama2$ (40)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Ama2$ (40)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$Ama2$ (40)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Ama2$ (40)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Ama2$ (40)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$Ama2$ (40)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Ama2$ (40)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Ama2$ (40)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Ama2$ (40)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Ama2$ (40)	$\langle 2;\ 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Cmcm$ (63); [2] $Cccm$ (66); [3] $P\bar{6}c2$ (188); [3] $P\bar{6}2c$ (190)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmm2$ (42)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pma2$ (28); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Amm2$ (38)

*Aea*2 No. 41 *Aea*2 C_{2v}^{17}

Former space-group symbol *Aba*2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$
8	*b*	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $A1a1$ (9, $C1c1$)	(1; 3)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,1/4,0$
[2] $Ae11$ (7, $P1c1$)	(1; 4)+	$1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a},\mathbf{b}$	$1/4,0,0$
[2] $A112$ (5)	(1; 2)+		

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pbn2_1$ (33, $Pna2_1$)	1; 4; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/4,0$
[2] $Pba2$ (32)	1; 2; 3; 4		
[2] $Pcn2$ (30, $Pnc2$)	1; 2; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Pca2_1$ (29)	1; 3; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$		$0,1/4,0$

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Aea2$ (41)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Aea2$ (41)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Aea2$ (41)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Aea2$ (41)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Aea2$ (41)	$\langle 2+(0,2,0);\ 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Aea2$ (41)	$\langle 2+(0,4,0);\ 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Aea2$ (41)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Aea2$ (41)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Aea2$ (41)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Aea2$ (41)	$\langle 2;\ 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] *Cmce* (64); [2] *Ccce* (68)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Fmm*2 (42)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ *Pma*2 (28); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ *Aem*2 (39)

C_{2v}^{18} $\quad Fmm2 \quad$ No. 42 $\quad Fmm2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+ \quad (\frac{1}{2},0,\frac{1}{2})+ \quad (\frac{1}{2},\frac{1}{2},0)+$
16	*e*	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $F1m1$ (8, $C1m1$)	(1; 3)+	$\mathbf{a},\mathbf{b},1/2(-\mathbf{a}+\mathbf{c})$	
[2] $Fm11$ (8, $C1m1$)	(1; 4)+	$\mathbf{c},\mathbf{a},1/2(\mathbf{b}-\mathbf{c})$	
[2] $F112$ (5, $A112$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Aea2$ (41)	1; 2; (1; 2) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $Bbe2$ (41, $Aea2$)	1; 2; (1; 2) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Ama2$ (40)	1; 4; (1; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$		1/4, 1/4, 0
[2] $Bbm2$ (40, $Ama2$)	1; 3; (1; 3) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 1/4, 0
[2] $Bme2$ (39, $Aem2$)	1; 4; (1; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 1/4, 0
[2] $Aem2$ (39)	1; 3; (1; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$		1/4, 1/4, 0
[2] $Amm2$ (38)	1; 2; 3; 4; (1; 2; 3; 4) + $(0,\frac{1}{2},\frac{1}{2})$		
[2] $Bmm2$ (38, $Amm2$)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},0,\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Ccc2$ (37)	1; 2; (1; 2) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4) + $(\frac{1}{2},0,\frac{1}{2})$		1/4, 1/4, 0
[2] $Ccm2_1$ (36, $Cmc2_1$)	1; 3; (1; 3) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4) + $(\frac{1}{2},0,\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 0, 0
[2] $Cmc2_1$ (36)	1; 4; (1; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 3) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3) + $(\frac{1}{2},0,\frac{1}{2})$		0, 1/4, 0
[2] $Cmm2$ (35)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},\frac{1}{2},0)$		

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$			
$Fmm2$ (42)	$\langle 2; 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Fmm2$ (42)	$\langle 3; 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$Fmm2$ (42)	$\langle 3; 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$Fmm2$ (42)	$\langle 2; 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Fmm2$ (42)	$\langle (2; 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$Fmm2$ (42)	$\langle (2; 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$Fmm2$ (42)	$\langle 2; 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$			
$Fmm2$ (42)	$\langle 3; 2+(2u,0,0)\rangle$ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	u, 0, 0
[p] $\mathbf{b}' = p\mathbf{b}$			
$Fmm2$ (42)	$\langle (2; 3)+(0,2u,0)\rangle$ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	0, u, 0
[p] $\mathbf{c}' = p\mathbf{c}$			
$Fmm2$ (42)	$\langle 2; 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Fmmm$ (69); [2] $I4mm$ (107); [2] $I4cm$ (108); [2] $I\bar{4}2m$ (121)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pmm2$ (25)

C_{2v}^{19} $\quad Fdd2 \quad$ No. 43 $\quad Fdd2$

Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+ \quad (\frac{1}{2},0,\frac{1}{2})+ \quad (\frac{1}{2},\frac{1}{2},0)+$
16	b	1	(1) x,y,z $\quad$ (2) $\bar{x},\bar{y},z$ $\quad$ (3) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$ $\quad$ (4) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $F1d1$ (9, $C1c1$)	(1; 3)+	$-\mathbf{c},\mathbf{b},1/2(\mathbf{a}+\mathbf{c})$	$0,1/8,0$
[2] $Fd11$ (9, $C1c1$)	(1; 4)+	$-\mathbf{b},\mathbf{a},1/2(\mathbf{b}+\mathbf{c})$	$1/8,0,0$
[2] $F112$ (5, $A112$)	(1; 2)+	$1/2(\mathbf{a}-\mathbf{b}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** $\quad$ none
- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Fdd2$ (43)	$\langle(2;\,3)+(\frac{1}{2},\frac{1}{2},0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1/4,1/4,0$
$Fdd2$ (43)	$\langle 2+(\frac{5}{2},\frac{1}{2},0);\, 3+(\frac{1}{2},\frac{1}{2},0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$5/4,1/4,0$
$Fdd2$ (43)	$\langle 2+(\frac{9}{2},\frac{1}{2},0);\, 3+(\frac{1}{2},\frac{1}{2},0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$9/4,1/4,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Fdd2$ (43)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\, 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$1/4,1/4,0$
$Fdd2$ (43)	$\langle 2+(\frac{1}{2},\frac{5}{2},0);\, 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$1/4,5/4,0$
$Fdd2$ (43)	$\langle 2+(\frac{1}{2},\frac{9}{2},0);\, 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$1/4,9/4,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Fdd2$ (43)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\, 3+(0,\frac{1}{2},\frac{1}{2})\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/4,1/4,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Fdd2$ (43)	$\langle 2+(\frac{1}{2}+2u,\frac{1}{2},0);\, 3+(\frac{p}{4}-\frac{1}{4},\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$1/4+u,1/4,0$
$Fdd2$ (43)	$\langle 2+(2u,0,0);\, 3+(\frac{p}{4}-\frac{1}{4},0,0)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Fdd2$ (43)	$\langle 2+(\frac{1}{2},\frac{1}{2}+2u,0);\, 3+(0,\frac{p}{4}+\frac{1}{4}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3 \pmod 4$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$1/4,1/4+u,0$
$Fdd2$ (43)	$\langle 2+(0,2u,0);\, 3+(0,\frac{p}{4}-\frac{1}{4}+2u,0)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Fdd2$ (43)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\, 3+(0,\frac{1}{2},\frac{p}{4}-\frac{1}{4})\rangle$ $p>2;\ p\equiv 3 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/4,1/4,0$
$Fdd2$ (43)	$\langle 2;\, 3+(0,0,\frac{p}{4}-\frac{1}{4})\rangle$ $p>4;\ p\equiv 1 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Fddd$ (70); [2] $I4_1md$ (109); [2] $I4_1cd$ (110); [2] $I\bar{4}2d$ (122)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** $\quad$ none
- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pnn2$ (34)

$Imm2$ No. 44 $Imm2$ C_{2v}^{20}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8	e	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $I1m1$ (8, $C1m1$)	(1; 3)+	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $Im11$ (8, $C1m1$)	(1; 4)+	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	
[2] $I112$ (5, $A112$)	(1; 2)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pnn2$ (34)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $Pnm2_1$ (31, $Pmn2_1$)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,0,0$
[2] $Pmn2_1$ (31)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/4,0$
[2] $Pmm2$ (25)	1; 2; 3; 4		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Imm2$ (44)	$\langle 2;\ 3\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Imm2$ (44)	$\langle 3;\ 2+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Imm2$ (44)	$\langle 3;\ 2+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Imm2$ (44)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Imm2$ (44)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Imm2$ (44)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Imm2$ (44)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Imm2$ (44)	$\langle 3;\ 2+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Imm2$ (44)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Imm2$ (44)	$\langle 2;\ 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Immm$ (71); [2] $Imma$ (74); [2] $I4mm$ (107); [2] $I4_1md$ (109); [2] $I\bar{4}m2$ (119)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Cmm2$ (35); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Amm2$ (38); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Bmm2$ (38, $Amm2$)

C_{2v}^{21} $Iba2$ No. 45 $Iba2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8 c 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $I1a1$ (9, $C1c1$)	(1; 3)+	$\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{c}$	
[2] $Ib11$ (9, $C1c1$)	(1; 4)+	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	
[2] $I112$ (5, $A112$)	(1; 2)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pba2$ (32)	1; 2; 3; 4		
[2] $Pca2_1$ (29)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 0
[2] $Pbc2_1$ (29, $Pca2_1$)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 1/4, 0
[2] $Pcc2$ (27)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Iba2$ (45)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Iba2$ (45)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$Iba2$ (45)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Iba2$ (45)	$\langle 2;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Iba2$ (45)	$\langle 2+(0,2,0);\ 3+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$Iba2$ (45)	$\langle 2+(0,4,0);\ 3+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Iba2$ (45)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Iba2$ (45)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Iba2$ (45)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Iba2$ (45)	$\langle 2;\ 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Ibam$ (72); [2] $Ibca$ (73); [2] $I4cm$ (108); [2] $I4_1cd$ (110); [2] $I\bar{4}c2$ (120)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Cmm2$ (35); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Aem2$ (39); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Bme2$ (39, $Aem2$)

$Ima2$ No. 46 $Ima2$ C_{2v}^{22}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x+\frac{1}{2},\bar{y},z$ (4) $\bar{x}+\frac{1}{2},y,z$

I Maximal *translationengleiche* subgroups

[2] $I1a1$ (9, $C1c1$)	(1; 3)+	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $Im11$ (8, $C1m1$)	(1; 4)+	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	1/4,0,0
[2] $I112$ (5, $A112$)	(1; 2)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pna2_1$ (33)	1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4,1/4,0
[2] $Pnc2$ (30)	1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $Pma2$ (28)	1; 2; 3; 4		
[2] $Pmc2_1$ (26)	1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4,1/4,0

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Ima2$ (46)	$\langle 2;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Ima2$ (46)	$\langle 2+(2,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1,0,0
$Ima2$ (46)	$\langle 2+(4,0,0);\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2,0,0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Ima2$ (46)	$\langle 2;\ 3\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Ima2$ (46)	$\langle (2;\ 3)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0,1,0
$Ima2$ (46)	$\langle (2;\ 3)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0,2,0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Ima2$ (46)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Ima2$ (46)	$\langle 2+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2},0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	u,0,0
[p] $\mathbf{b}'=p\mathbf{b}$			
$Ima2$ (46)	$\langle (2;\ 3)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	0,u,0
[p] $\mathbf{c}'=p\mathbf{c}$			
$Ima2$ (46)	$\langle 2;\ 3\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

I Minimal *translationengleiche* supergroups

[2] $Ibam$ (72); [2] $Imma$ (74)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Cmm2$ (35); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Amm2$ (38); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Bme2$ (39, $Aem2$)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 47, pp. 153–154.

D_{2h}^1 $P2/m2/m2/m$ No. 47   *Pmmm*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] *Pmm*2 (25)	1; 2; 7; 8	
[2] *Pm*2*m* (25, *Pmm*2)	1; 3; 6; 8	**c**, **a**, **b**
[2] *P*2*mm* (25, *Pmm*2)	1; 4; 6; 7	**b**, **c**, **a**
[2] *P*222 (16)	1; 2; 3; 4	
[2] *P*112/*m* (10)	1; 2; 5; 6	
[2] *P*12/*m*1 (10)	1; 3; 5; 7	
[2] *P*2/*m*11 (10, *P*12/*m*1)	1; 4; 5; 8	**c**, **a**, **b**

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}' = 2\mathbf{a}$			
Pmma (51)	⟨3; 5; 2 + (1,0,0)⟩	2**a**, **b**, **c**	
Pmma (51)	⟨2; (3; 5) + (1,0,0)⟩	2**a**, **b**, **c**	1/2, 0, 0
Pmam (51, *Pmma*)	⟨2; 5; 3 + (1,0,0)⟩	2**a**, −**c**, **b**	
Pmam (51, *Pmma*)	⟨3; (2; 5) + (1,0,0)⟩	2**a**, −**c**, **b**	1/2, 0, 0
Pmaa (49, *Pccm*)	⟨5; (2; 3) + (1,0,0)⟩	**b**, **c**, 2**a**	
Pmaa (49, *Pccm*)	⟨2; 3; 5 + (1,0,0)⟩	**b**, **c**, 2**a**	1/2, 0, 0
Pmmm (47)	⟨2; 3; 5⟩	2**a**, **b**, **c**	
Pmmm (47)	⟨(2; 3; 5) + (1,0,0)⟩	2**a**, **b**, **c**	1/2, 0, 0
[2] $\mathbf{b}' = 2\mathbf{b}$			
Pbmm (51, *Pmma*)	⟨2; 5; 3 + (0,1,0)⟩	2**b**, **c**, **a**	
Pbmm (51, *Pmma*)	⟨(2; 3; 5) + (0,1,0)⟩	2**b**, **c**, **a**	0, 1/2, 0
Pmmb (51, *Pmma*)	⟨5; (2; 3) + (0,1,0)⟩	−2**b**, **a**, **c**	
Pmmb (51, *Pmma*)	⟨2; (3; 5) + (0,1,0)⟩	−2**b**, **a**, **c**	0, 1/2, 0
Pbmb (49, *Pccm*)	⟨3; 5; 2 + (0,1,0)⟩	**c**, **a**, 2**b**	
Pbmb (49, *Pccm*)	⟨2; 3; 5 + (0,1,0)⟩	**c**, **a**, 2**b**	0, 1/2, 0
Pmmm (47)	⟨2; 3; 5⟩	**a**, 2**b**, **c**	
Pmmm (47)	⟨3; (2; 5) + (0,1,0)⟩	**a**, 2**b**, **c**	0, 1/2, 0
[2] $\mathbf{c}' = 2\mathbf{c}$			
Pcmm (51, *Pmma*)	⟨3; 5; 2 + (0,0,1)⟩	2**c**, **b**, −**a**	
Pcmm (51, *Pmma*)	⟨(2; 3; 5) + (0,0,1)⟩	2**c**, **b**, −**a**	0, 0, 1/2
Pmcm (51, *Pmma*)	⟨5; (2; 3) + (0,0,1)⟩	2**c**, **a**, **b**	
Pmcm (51, *Pmma*)	⟨3; (2; 5) + (0,0,1)⟩	2**c**, **a**, **b**	0, 0, 1/2
Pccm (49)	⟨2; 5; 3 + (0,0,1)⟩	**a**, **b**, 2**c**	
Pccm (49)	⟨2; 3; 5 + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
Pmmm (47)	⟨2; 3; 5⟩	**a**, **b**, 2**c**	
Pmmm (47)	⟨2; (3; 5) + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$			
Aemm (67, *Cmme*)	⟨3; 5; 2 + (0,0,1)⟩	2**b**, 2**c**, **a**	
Aemm (67, *Cmme*)	⟨(2; 3; 5) + (0,0,1)⟩	2**b**, 2**c**, **a**	0, 0, 1/2
Aemm (67, *Cmme*)	⟨2; 5; 3 + (0,0,1)⟩	2**b**, 2**c**, **a**	0, 1/2, 1/2
Aemm (67, *Cmme*)	⟨2; 3; 5 + (0,0,1)⟩	2**b**, 2**c**, **a**	0, 1/2, 0
Ammm (65, *Cmmm*)	⟨2; 3; 5⟩	2**b**, 2**c**, **a**	
Ammm (65, *Cmmm*)	⟨2; (3; 5) + (0,0,1)⟩	2**b**, 2**c**, **a**	0, 0, 1/2
Ammm (65, *Cmmm*)	⟨5; (2; 3) + (0,0,1)⟩	2**b**, 2**c**, **a**	0, 1/2, 1/2
Ammm (65, *Cmmm*)	⟨3; (2; 5) + (0,0,1)⟩	2**b**, 2**c**, **a**	0, 1/2, 0
[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$			
Bmem (67, *Cmme*)	⟨2; 5; 3 + (1,0,0)⟩	2**c**, 2**a**, **b**	
Bmem (67, *Cmme*)	⟨3; (2; 5) + (1,0,0)⟩	2**c**, 2**a**, **b**	1/2, 0, 0
Bmem (67, *Cmme*)	⟨5; (2; 3) + (1,0,0)⟩	2**c**, 2**a**, **b**	1/2, 0, 1/2
Bmem (67, *Cmme*)	⟨2; 3; 5 + (1,0,0)⟩	2**c**, 2**a**, **b**	0, 0, 1/2
Bmmm (65, *Cmmm*)	⟨2; 3; 5⟩	2**c**, 2**a**, **b**	
Bmmm (65, *Cmmm*)	⟨(2; 3; 5) + (1,0,0)⟩	2**c**, 2**a**, **b**	1/2, 0, 0
Bmmm (65, *Cmmm*)	⟨3; 5; 2 + (1,0,0)⟩	2**c**, 2**a**, **b**	1/2, 0, 1/2
Bmmm (65, *Cmmm*)	⟨2; (3; 5) + (1,0,0)⟩	2**c**, 2**a**, **b**	0, 0, 1/2

[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
Cmme (67)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 1/2, 0$
Cmme (67)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0, 1/2, 0$
Cmme (67)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
Cmme (67)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 0, 0$
Cmmm (65)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	
Cmmm (65)	$\langle (2;\ 3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 0, 0$
Cmmm (65)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$1/2, 1/2, 0$
Cmmm (65)	$\langle 3;\ (2;\ 5)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$0, 1/2, 0$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
Fmmm (69)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	
Fmmm (69)	$\langle (2;\ 3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 0, 0$
Fmmm (69)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 0, 1/2$
Fmmm (69)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0, 0, 1/2$
Fmmm (69)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 1/2, 0$
Fmmm (69)	$\langle 3;\ (2;\ 5)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0, 1/2, 0$
Fmmm (69)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0, 1/2, 1/2$
Fmmm (69)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2, 1/2, 1/2$
[3] $\mathbf{a}' = 3\mathbf{a}$			
Pmmm (47)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
Pmmm (47)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1, 0, 0$
Pmmm (47)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$2, 0, 0$
[3] $\mathbf{b}' = 3\mathbf{b}$			
Pmmm (47)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
Pmmm (47)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 1, 0$
Pmmm (47)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 2, 0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
Pmmm (47)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
Pmmm (47)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 1$
Pmmm (47)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
Pmmm (47)	$\langle (2;\ 3;\ 5)+(2u,0,0)\rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
Pmmm (47)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
Pmmm (47)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4_2/mmc$ (131); [3] $Pm\bar{3}$ (200)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Ammm* (65, *Cmmm*); [2] *Bmmm* (65, *Cmmm*); [2] *Cmmm* (65); [2] *Immm* (71)

- **Decreased unit cell** none

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 48, pp. 155–157.

D_{2h}^2 $P2/n2/n2/n$ No. 48 $Pnnn$

ORIGIN CHOICE 1, Origin at 222, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	m	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Pnn2$ (34)	1; 2; 7; 8		
[2] $Pn2n$ (34, $Pnn2$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $P2nn$ (34, $Pnn2$)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $P222$ (16)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 1/4, 1/4
[2] $P12/n1$ (13, $P12/c1$)	1; 3; 5; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	1/4, 1/4, 1/4
[2] $P2/n11$ (13, $P12/c1$)	1; 4; 5; 8	$-\mathbf{b},\mathbf{a},\mathbf{b}+\mathbf{c}$	1/4, 1/4, 1/4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$Fddd$ (70)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fddd$ (70)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	0, 0, 1/2
$Fddd$ (70)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 0, 0
$Fddd$ (70)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	0, 1/2, 0
$Fddd$ (70)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 1/2, 0
$Fddd$ (70)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 0, 1/2
$Fddd$ (70)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	0, 1/2, 1/2
$Fddd$ (70)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 1/2, 1/2
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pnnn$ (48)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pnnn$ (48)	$\langle (2;\ 3)+(2,0,0);\ 5+(3,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$Pnnn$ (48)	$\langle (2;\ 3)+(4,0,0);\ 5+(5,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pnnn$ (48)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pnnn$ (48)	$\langle 3;\ 2+(0,2,0);\ 5+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$Pnnn$ (48)	$\langle 3;\ 2+(0,4,0);\ 5+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pnnn$ (48)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pnnn$ (48)	$\langle 2;\ 3+(0,0,2);\ 5+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$Pnnn$ (48)	$\langle 2;\ 3+(0,0,4);\ 5+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Pnnn$ (48)	$\langle (2;\ 3)+(2u,0,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Pnnn$ (48)	$\langle 3;\ 2+(0,2u,0);\ 5+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Pnnn$ (48)	$\langle 2;\ 3+(0,0,2u);\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/nnc$ (126); [2] $P4_2/nnm$ (134); [3] $Pn\bar{3}$ (201)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Immm* (71); [2] *Amaa* (66, *Cccm*); [2] *Bbmb* (66, *Cccm*); [2] *Cccm* (66)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pncb* (50, *Pban*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pcna* (50, *Pban*); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Pban* (50)

Pnnn ORIGIN CHOICE 2 No. 48

(*Continued from the facing page*)

I Minimal *translationengleiche* supergroups

[2] $P4/nnc$ (126); [2] $P4_2/nnm$ (134); [3] $Pn\bar{3}$ (201)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Immm* (71); [2] *Amaa* (66, *Cccm*); [2] *Bbmb* (66, *Cccm*); [2] *Cccm* (66)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pncb* (50, *Pban*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pcna* (50, *Pban*); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Pban* (50)

ORIGIN CHOICE 2, Origin at $\bar{1}$ at nnn, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from 222

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	m	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Pnn2$ (34)	1; 2; 7; 8		$1/4,1/4,1/4$
[2] $Pn2n$ (34, $Pnn2$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,1/4$
[2] $P2nn$ (34, $Pnn2$)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,1/4,1/4$
[2] $P222$ (16)	1; 2; 3; 4		$1/4,1/4,1/4$
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P12/n1$ (13, $P12/c1$)	1; 3; 5; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2] $P2/n11$ (13, $P12/c1$)	1; 4; 5; 8	$-\mathbf{b},\mathbf{a},\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$Fddd$ (70)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fddd$ (70)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$Fddd$ (70)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,0,0$
$Fddd$ (70)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$Fddd$ (70)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$Fddd$ (70)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,0,1/2$
$Fddd$ (70)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$Fddd$ (70)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Pnnn$ (48)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Pnnn$ (48)	$\langle (2;\ 3)+(3,0,0);\ 5+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Pnnn$ (48)	$\langle (2;\ 3)+(5,0,0);\ 5+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Pnnn$ (48)	$\langle 3;\ 5;\ 2+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Pnnn$ (48)	$\langle 3;\ 2+(0,3,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Pnnn$ (48)	$\langle 3;\ 2+(0,5,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $Pnnn$ (48)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $Pnnn$ (48)	$\langle 2;\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $Pnnn$ (48)	$\langle 2;\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pnnn$ (48)	$\langle (2;\ 3)+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pnnn$ (48)	$\langle 3;\ 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 5+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pnnn$ (48)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

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International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 49, pp. 158–159.

$Pccm$ No. 49 $P2/c2/c2/m$ D_{2h}^{3}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
8	r	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x,\bar{y},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x,y,\bar{z}$ (7) $x,\bar{y},z+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Pc2m$ (28, $Pma2$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $P2cm$ (28, $Pma2$)	1; 4; 6; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,0,1/4$
[2] $Pcc2$ (27)	1; 2; 7; 8		
[2] $P222$ (16)	1; 2; 3; 4		$0,0,1/4$
[2] $P12/c1$ (13)	1; 3; 5; 7		
[2] $P2/c11$ (13, $P12/c1$)	1; 4; 5; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P112/m$ (10)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$Pcca$ (54)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pcca$ (54)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Pcnm$ (53, $Pmna$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{c},\mathbf{b},-2\mathbf{a}$	
$Pcnm$ (53, $Pmna$)	$\langle 3;\ (2;\ 5)+(1,0,0)\rangle$	$\mathbf{c},\mathbf{b},-2\mathbf{a}$	$1/2,0,0$
$Pcna$ (50, $Pban$)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$\mathbf{c},2\mathbf{a},\mathbf{b}$	
$Pcna$ (50, $Pban$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{c},2\mathbf{a},\mathbf{b}$	$1/2,0,0$
$Pccm$ (49)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pccm$ (49)	$\langle (2;\ 3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $\mathbf{b}'=2\mathbf{b}$			
$Pccb$ (54, $Pcca$)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$-2\mathbf{b},\mathbf{a},\mathbf{c}$	
$Pccb$ (54, $Pcca$)	$\langle 2;\ (3;\ 5)+(0,1,0)\rangle$	$-2\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/2,0$
$Pncm$ (53, $Pmna$)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	
$Pncm$ (53, $Pmna$)	$\langle (2;\ 3;\ 5)+(0,1,0)\rangle$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	$0,1/2,0$
$Pncb$ (50, $Pban$)	$\langle 3;\ 5;\ 2+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	
$Pncb$ (50, $Pban$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/2,0$
$Pccm$ (49)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pccm$ (49)	$\langle 3;\ (2;\ 5)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$Ccce$ (68)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Ccce$ (68)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$Ccce$ (68)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$Ccce$ (68)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Cccm$ (66)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Cccm$ (66)	$\langle (2;\ 3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Cccm$ (66)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$Cccm$ (66)	$\langle 3;\ (2;\ 5)+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
$\{$ $Pccm$ (49)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pccm$ (49)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pccm$ (49)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$\{$ $Pccm$ (49)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pccm$ (49)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pccm$ (49)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$\{$ $Pccm$ (49)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pccm$ (49)	$\langle 2;\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pccm$ (49)	$\langle 2;\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$

$Pccm$ (49)	$\langle(2;\ 3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$

[p] $\mathbf{b}' = p\mathbf{b}$

$Pccm$ (49)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$

[p] $\mathbf{c}' = p\mathbf{c}$

$Pccm$ (49)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/mcc$ (124); [2] $P4_2/mcm$ (132)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cccm$ (66); [2] $Aemm$ (67, $Cmme$); [2] $Bmem$ (67, $Cmme$); [2] $Ibam$ (72)

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pmmm$ (47)

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I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmmm$ (65); [2] $Aeaa$ (68, $Ccce$); [2] $Bbeb$ (68, $Ccce$); [2] $Ibam$ (72)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pbmb$ (49, $Pccm$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmaa$ (49, $Pccm$)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 50, pp. 159–162.

Pban No. 50 $P2/b2/a2/n$ D_{2h}^4

ORIGIN CHOICE 1, Origin at $222/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*m*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] *Pba*2 (32)	1; 2; 7; 8		
[2] *Pb*2*n* (30, *Pnc*2)	1; 3; 6; 8	**c**, **a**, **b**	
[2] *P*2*an* (30, *Pnc*2)	1; 4; 6; 7	**c**, **b**, −**a**	
[2] *P*222 (16)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	−**a** − **b**, **a**, **c**	1/4, 1/4, 0
[2] $P12/a1$ (13, $P12/c1$)	1; 3; 5; 7	−**a** − **c**, **b**, **a**	1/4, 1/4, 0
[2] $P2/b11$ (13, $P12/c1$)	1; 4; 5; 8	**c**, **a**, **b**	1/4, 1/4, 0

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
Pnan (52, *Pnna*)	⟨3; 5; 2 + (0,0,1)⟩	**a**, −2**c**, **b**	1/4, 1/4, 0
Pnan (52, *Pnna*)	⟨(2; 3; 5) + (0,0,1)⟩	**a**, −2**c**, **b**	1/4, 1/4, 1/2
Pbnn (52, *Pnna*)	⟨5; (2; 3) + (0,0,1)⟩	**b**, 2**c**, **a**	1/4, 1/4, 0
Pbnn (52, *Pnna*)	⟨3; (2; 5) + (0,0,1)⟩	**b**, 2**c**, **a**	1/4, 1/4, 1/2
Pban (50)	⟨2; 3; 5⟩	**a**, **b**, 2**c**	
Pban (50)	⟨2; (3; 5) + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
Pnnn (48)	⟨2; 5; 3 + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
Pnnn (48)	⟨2; 3; 5 + (0,0,1)⟩	**a**, **b**, 2**c**	
[3] $\mathbf{a}' = 3\mathbf{a}$			
{ *Pban* (50)	⟨2; 3; 5 + (1,0,0)⟩	3**a**, **b**, **c**	
{ *Pban* (50)	⟨(2; 3) + (2,0,0); 5 + (3,0,0)⟩	3**a**, **b**, **c**	1, 0, 0
{ *Pban* (50)	⟨(2; 3) + (4,0,0); 5 + (5,0,0)⟩	3**a**, **b**, **c**	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
{ *Pban* (50)	⟨2; 3; 5 + (0,1,0)⟩	**a**, 3**b**, **c**	
{ *Pban* (50)	⟨3; 2 + (0,2,0); 5 + (0,3,0)⟩	**a**, 3**b**, **c**	0, 1, 0
{ *Pban* (50)	⟨3; 2 + (0,4,0); 5 + (0,5,0)⟩	**a**, 3**b**, **c**	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
{ *Pban* (50)	⟨2; 3; 5⟩	**a**, **b**, 3**c**	
{ *Pban* (50)	⟨2; (3; 5) + (0,0,2)⟩	**a**, **b**, 3**c**	0, 0, 1
{ *Pban* (50)	⟨2; (3; 5) + (0,0,4)⟩	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$			
Pban (50)	$\langle(2;\ 3) + (2u,0,0);\ 5 + (\frac{p}{2} - \frac{1}{2} + 2u,0,0)\rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	p**a**, **b**, **c**	u, 0, 0
[p] $\mathbf{b}' = p\mathbf{b}$			
Pban (50)	$\langle 3;\ 2 + (0,2u,0);\ 5 + (0,\frac{p}{2} - \frac{1}{2} + 2u,0)\rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	**a**, p**b**, **c**	0, u, 0
[p] $\mathbf{c}' = p\mathbf{c}$			
Pban (50)	$\langle 2;\ (3;\ 5) + (0,0,2u)\rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	**a**, **b**, p**c**	0, 0, u

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ORIGIN CHOICE 2, Origin at $\bar{1}$ at ban, at $-\frac{1}{4},-\frac{1}{4},0$ from 222

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	m	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $x+\frac{1}{2},\bar{y},z$	(8) $\bar{x},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $Pba2$ (32)	1; 2; 7; 8		$1/4,1/4,0$
[2] $Pb2n$ (30, $Pnc2$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
[2] $P2an$ (30, $Pnc2$)	1; 4; 6; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$1/4,1/4,0$
[2] $P222$ (16)	1; 2; 3; 4		$1/4,1/4,0$
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P12/a1$ (13, $P12/c1$)	1; 3; 5; 7	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $P2/b11$ (13, $P12/c1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$Pnan$ (52, $Pnna$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$\mathbf{a},-2\mathbf{c},\mathbf{b}$	
$Pnan$ (52, $Pnna$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},-2\mathbf{c},\mathbf{b}$	$0,0,1/2$
$Pbnn$ (52, $Pnna$)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{b},2\mathbf{c},\mathbf{a}$	
$Pbnn$ (52, $Pnna$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,0,1/2$
$Pban$ (50)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pban$ (50)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$Pnnn$ (48)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pnnn$ (48)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pban$ (50)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pban$ (50)	$\langle (2;\ 3)+(3,0,0);\ 5+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pban$ (50)	$\langle (2;\ 3)+(5,0,0);\ 5+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pban$ (50)	$\langle 3;\ 5;\ 2+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pban$ (50)	$\langle 3;\ 2+(0,3,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pban$ (50)	$\langle 3;\ 2+(0,5,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pban$ (50)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pban$ (50)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pban$ (50)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pban$ (50)	$\langle (2;\ 3)+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pban$ (50)	$\langle 3;\ 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 5+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pban$ (50)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4_2/nbc$ (133)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Cmmm* (65); [2] *Aeaa* (68, *Ccce*); [2] *Bbeb* (68, *Ccce*); [2] *Ibam* (72)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pbmb* (49, *Pccm*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pmaa* (49, *Pccm*)

Pmma No. 51

(*Continued from the facing page*)

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
Pmma (51)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
Pmma (51)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
Pmma (51)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Amma* (63, *Cmcm*); [2] *Bmmm* (65, *Cmmm*); [2] *Cmme* (67); [2] *Imma* (74)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pmmm* (47)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 51, pp. 162–163.

D_{2h}^{5} $P2_1/m2/m2/a$ No. 51 *Pmma*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
8	l	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x+\frac{1}{2},\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x+\frac{1}{2},y,\bar{z}$ (7) $x,\bar{y},z$ (8) $\bar{x}+\frac{1}{2},y,z$

I Maximal *translationengleiche* subgroups

[2] $Pm2a$ (28, $Pma2$)	1; 3; 6; 8	$\mathbf{a},-\mathbf{c},\mathbf{b}$	
[2] $P2_1ma$ (26, $Pmc2_1$)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pmm2$ (25)	1; 2; 7; 8		$1/4,0,0$
[2] $P2_122$ (17, $P222_1$)	1; 2; 3; 4	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $P112/a$ (13)	1; 2; 5; 6		
[2] $P2_1/m11$ (11, $P12_1/m1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $P12/m1$ (10)	1; 3; 5; 7		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$Pmmn$ (59)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$Pbma$ (57, $Pbcm$)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	
$Pbma$ (57, $Pbcm$)	$\langle (2;\ 3;\ 5)+(0,1,0)\rangle$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	$0,1/2,0$
$Pbmn$ (53, $Pmna$)	$\langle 3;\ 5;\ 2+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	
$Pbmn$ (53, $Pmna$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/2,0$
$Pmma$ (51)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pmma$ (51)	$\langle 3;\ (2;\ 5)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $\mathbf{c}'=2\mathbf{c}$			
$Pmca$ (57, $Pbcm$)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{b},2\mathbf{c},\mathbf{a}$	
$Pmca$ (57, $Pbcm$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,0,1/2$
$Pcma$ (55, $Pbam$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	
$Pcma$ (55, $Pbam$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/2$
$Pcca$ (54)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pcca$ (54)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$Pmma$ (51)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pmma$ (51)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{b}'=2\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$Aema$ (64, $Cmce$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	
$Aema$ (64, $Cmce$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,0,1/2$
$Aema$ (64, $Cmce$)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,1/2,1/2$
$Aema$ (64, $Cmce$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,1/2,0$
$Amma$ (63, $Cmcm$)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	
$Amma$ (63, $Cmcm$)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,0,1/2$
$Amma$ (63, $Cmcm$)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,1/2,1/2$
$Amma$ (63, $Cmcm$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$2\mathbf{b},2\mathbf{c},\mathbf{a}$	$0,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pmma$ (51)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pmma$ (51)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pmma$ (51)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pmma$ (51)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pmma$ (51)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pmma$ (51)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pmma$ (51)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pmma$ (51)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pmma$ (51)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

(*Continued on the facing page*)

Pnna No. 52 $P2/n2_1/n2/a$ D_{2h}^6

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*e*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}$	(7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] *Pnn*2 (34)	1; 2; 7; 8		1/4, 0, 0
[2] $Pn2_1a$ (33, $Pna2_1$)	1; 3; 6; 8	$\mathbf{a},-\mathbf{c},\mathbf{b}$	1/4, 0, 1/4
[2] *P*2*na* (30, *Pnc*2)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	0, 1/4, 1/4
[2] $P22_12$ (17, $P222_1$)	1; 2; 3; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 0, 1/4
[2] $P12_1/n1$ (14, $P12_1/c1$)	1; 3; 5; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2] $P112/a$ (13)	1; 2; 5; 6		
[2] $P2/n11$ (13, $P12/c1$)	1; 4; 5; 8	$-\mathbf{b},\mathbf{a},\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
Pnna (52)	⟨5; (2; 3) + (1, 0, 0)⟩	3**a**, **b**, **c**	
Pnna (52)	⟨(2; 3) + (3, 0, 0); 5 + (2, 0, 0)⟩	3**a**, **b**, **c**	1, 0, 0
Pnna (52)	⟨(2; 3) + (5, 0, 0); 5 + (4, 0, 0)⟩	3**a**, **b**, **c**	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
Pnna (52)	⟨2; 5; 3 + (0, 1, 0)⟩	**a**, 3**b**, **c**	
Pnna (52)	⟨(2; 5) + (0, 2, 0); 3 + (0, 1, 0)⟩	**a**, 3**b**, **c**	0, 1, 0
Pnna (52)	⟨(2; 5) + (0, 4, 0); 3 + (0, 1, 0)⟩	**a**, 3**b**, **c**	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
Pnna (52)	⟨2; 5; 3 + (0, 0, 1)⟩	**a**, **b**, 3**c**	
Pnna (52)	⟨2; 3 + (0, 0, 3); 5 + (0, 0, 2)⟩	**a**, **b**, 3**c**	0, 0, 1
Pnna (52)	⟨2; 3 + (0, 0, 5); 5 + (0, 0, 4)⟩	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

[*p*] $\mathbf{a}'=p\mathbf{a}$			
Pnna (52)	$\langle(2;\ 3)+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ *p* conjugate subgroups for the prime *p*	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[*p*] $\mathbf{b}'=p\mathbf{b}$			
Pnna (52)	$\langle(2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ *p* conjugate subgroups for the prime *p*	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[*p*] $\mathbf{c}'=p\mathbf{c}$			
Pnna (52)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ *p* conjugate subgroups for the prime *p*	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Bbmm* (63, *Cmcm*); [2] *Amaa* (66, *Cccm*); [2] *Ccce* (68); [2] *Imma* (74)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ *Pncm* (53, *Pmna*); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ *Pcna* (50, *Pban*); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ *Pbaa* (54, *Pcca*)

D_{2h}^{7} $P2/m2/n2_1/a$ No. 53 $Pmna$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*i*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $Pmn2_1$ (31)	1; 2; 7; 8		
[2] $P2na$ (30, $Pnc2$)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pm2a$ (28, $Pma2$)	1; 3; 6; 8	$\mathbf{a},-\mathbf{c},\mathbf{b}$	$1/4,0,1/4$
[2] $P222_1$ (17)	1; 2; 3; 4		$1/4,0,0$
[2] $P112_1/a$ (14)	1; 2; 5; 6		
[2] $P12/n1$ (13, $P12/c1$)	1; 3; 5; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2] $P2/m11$ (10, $P12/m1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
$Pbna$ (60, $Pbcn$)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	
$Pbna$ (60, $Pbcn$)	$\langle (2;\ 3;\ 5)+(0,1,0)\rangle$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	$0,1/2,0$
$Pmnn$ (58, $Pnnm$)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	
$Pmnn$ (58, $Pnnm$)	$\langle 2;\ (3;\ 5)+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/2,0$
$Pmna$ (53)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	
$Pmna$ (53)	$\langle 3;\ (2;\ 5)+(0,1,0)\rangle$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1/2,0$
$Pbnn$ (52, $Pnna$)	$\langle 3;\ 5;\ 2+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	
$Pbnn$ (52, $Pnna$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/2,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
{ $Pmna$ (53)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
{ $Pmna$ (53)	$\langle (2;\ 3)+(3,0,0);\ 5+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
{ $Pmna$ (53)	$\langle (2;\ 3)+(5,0,0);\ 5+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
{ $Pmna$ (53)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
{ $Pmna$ (53)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
{ $Pmna$ (53)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $Pmna$ (53)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $Pmna$ (53)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $Pmna$ (53)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pmna$ (53)	$\langle (2;\ 3)+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 5+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pmna$ (53)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pmna$ (53)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmce$ (64); [2] $Bmmm$ (65, $Cmmm$); [2] $Amaa$ (66, $Cccm$); [2] $Imma$ (74)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pmaa$ (49, $Pccm$); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pmcm$ (51, $Pmma$)

Pcca No. 54 $P2_1/c2/c2/a$ D_{2h}^8

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*f*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] *Pc*2*a* (32, *Pba*2)	1; 3; 6; 8	**a**, −**c**, **b**	0, 0, 1/4
[2] $P2_1ca$ (29, $Pca2_1$)	1; 4; 6; 7	**c**, **b**, −**a**	0, 0, 1/4
[2] *Pcc*2 (27)	1; 2; 7; 8		1/4, 0, 0
[2] $P2_122$ (17, $P222_1$)	1; 2; 3; 4	**b**, **c**, **a**	0, 0, 1/4
[2] $P2_1/c11$ (14, $P12_1/c1$)	1; 4; 5; 8	−**b**, **a**, **c**	
[2] $P112/a$ (13)	1; 2; 5; 6		
[2] $P12/c1$ (13)	1; 3; 5; 7		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{b}'=2\mathbf{b}$			
Pnca (60, *Pbcn*)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	2**b**, **c**, **a**	
Pnca (60, *Pbcn*)	$\langle (2;\ 3;\ 5)+(0,1,0)\rangle$	2**b**, **c**, **a**	0, 1/2, 0
Pccn (56)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	**a**, 2**b**, **c**	
Pccn (56)	$\langle 2;\ (3;\ 5)+(0,1,0)\rangle$	**a**, 2**b**, **c**	0, 1/2, 0
Pcca (54)	$\langle 2;\ 3;\ 5\rangle$	**a**, 2**b**, **c**	
Pcca (54)	$\langle 3;\ (2;\ 5)+(0,1,0)\rangle$	**a**, 2**b**, **c**	0, 1/2, 0
Pncn (52, *Pnna*)	$\langle 3;\ 5;\ 2+(0,1,0)\rangle$	**c**, **a**, 2**b**	
Pncn (52, *Pnna*)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	**c**, **a**, 2**b**	0, 1/2, 0
[3] $\mathbf{a}'=3\mathbf{a}$			
Pcca (54)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	3**a**, **b**, **c**	
Pcca (54)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	3**a**, **b**, **c**	1, 0, 0
Pcca (54)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	3**a**, **b**, **c**	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
Pcca (54)	$\langle 2;\ 3;\ 5\rangle$	**a**, 3**b**, **c**	
Pcca (54)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	**a**, 3**b**, **c**	0, 1, 0
Pcca (54)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	**a**, 3**b**, **c**	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
Pcca (54)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	**a**, **b**, 3**c**	
Pcca (54)	$\langle 2;\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	**a**, **b**, 3**c**	0, 0, 1
Pcca (54)	$\langle 2;\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

[*p*] $\mathbf{a}'=p\mathbf{a}$			
Pcca (54)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2$; $0\leq u<p$ *p* conjugate subgroups for the prime *p*	*p***a**, **b**, **c**	*u*, 0, 0
[*p*] $\mathbf{b}'=p\mathbf{b}$			
Pcca (54)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2$; $0\leq u<p$ *p* conjugate subgroups for the prime *p*	**a**, *p***b**, **c**	0, *u*, 0
[*p*] $\mathbf{c}'=p\mathbf{c}$			
Pcca (54)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2$; $0\leq u<p$ *p* conjugate subgroups for the prime *p*	**a**, **b**, *p***c**	0, 0, *u*

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Aema* (64, *Cmce*); [2] *Bmem* (67, *Cmme*); [2] *Ccce* (68); [2] *Ibca* (73)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ *Pccm* (49); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ *Pmma* (51)

D_{2h}^{9} $P2_1/b2_1/a2/m$ No. 55 $Pbam$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $Pba2$ (32)	1; 2; 7; 8		
[2] $Pb2_1m$ (26, $Pmc2_1$)	1; 3; 6; 8	**c**, **a**, **b**	1/4, 0, 0
[2] $P2_1am$ (26, $Pmc2_1$)	1; 4; 6; 7	**c**, **b**, −**a**	0, 1/4, 0
[2] $P2_12_12$ (18)	1; 2; 3; 4		
[2] $P12_1/a1$ (14, $P12_1/c1$)	1; 3; 5; 7	−**a** − **c**, **b**, **a**	
[2] $P2_1/b11$ (14, $P12_1/c1$)	1; 4; 5; 8	**c**, **a**, **b**	
[2] $P112/m$ (10)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$Pnam$ (62, $Pnma$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	**a**, −2**c**, **b**	
$Pnam$ (62, $Pnma$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	**a**, −2**c**, **b**	0, 0, 1/2
$Pbnm$ (62, $Pnma$)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	**b**, 2**c**, **a**	
$Pbnm$ (62, $Pnma$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	**b**, 2**c**, **a**	0, 0, 1/2
$Pnnm$ (58)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	**a**, **b**, 2**c**	
$Pnnm$ (58)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	**a**, **b**, 2**c**	0, 0, 1/2
$Pbam$ (55)	$\langle 2;\ 3;\ 5\rangle$	**a**, **b**, 2**c**	
$Pbam$ (55)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	**a**, **b**, 2**c**	0, 0, 1/2
[3] $\mathbf{a}' = 3\mathbf{a}$			
$Pbam$ (55)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	3**a**, **b**, **c**	
$Pbam$ (55)	$\langle (2;\ 5)+(2,0,0);\ 3+(3,0,0)\rangle$	3**a**, **b**, **c**	1, 0, 0
$Pbam$ (55)	$\langle (2;\ 5)+(4,0,0);\ 3+(5,0,0)\rangle$	3**a**, **b**, **c**	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$Pbam$ (55)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	
$Pbam$ (55)	$\langle (2;\ 5)+(0,2,0);\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	0, 1, 0
$Pbam$ (55)	$\langle (2;\ 5)+(0,4,0);\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$Pbam$ (55)	$\langle 2;\ 3;\ 5\rangle$	**a**, **b**, 3**c**	
$Pbam$ (55)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	**a**, **b**, 3**c**	0, 0, 1
$Pbam$ (55)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$			
$Pbam$ (55)	$\langle (2;\ 5)+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	p**a**, **b**, **c**	u, 0, 0
[p] $\mathbf{b}' = p\mathbf{b}$			
$Pbam$ (55)	$\langle (2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	**a**, p**b**, **c**	0, u, 0
[p] $\mathbf{c}' = p\mathbf{c}$			
$Pbam$ (55)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	**a**, **b**, p**c**	0, 0, u

I Minimal *translationengleiche* supergroups

[2] $P4/mbm$ (127); [2] $P4_2/mbc$ (135)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Aeam$ (64, $Cmce$); [2] $Bbem$ (64, $Cmce$); [2] $Cmmm$ (65); [2] $Ibam$ (72)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Pbmm$ (51, $Pmma$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmam$ (51, $Pmma$)

$Pccn$ No. 56 $P2_1/c2_1/c2/n$ D_{2h}^{10}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
8	e	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Pc2_1n$ (33, $Pna2_1$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $P2_1cn$ (33, $Pna2_1$)	1; 4; 6; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,0,1/4$
[2] $Pcc2$ (27)	1; 2; 7; 8		$1/4,1/4,0$
[2] $P2_12_12$ (18)	1; 2; 3; 4		$1/4,1/4,1/4$
[2] $P12_1/c1$ (14)	1; 3; 5; 7		
[2] $P2_1/c11$ (14, $P12_1/c1$)	1; 4; 5; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Pccn$ (56)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pccn$ (56)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pccn$ (56)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pccn$ (56)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pccn$ (56)	$\langle 2+(0,3,0);\ 3+(0,1,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pccn$ (56)	$\langle 2+(0,5,0);\ 3+(0,1,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pccn$ (56)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pccn$ (56)	$\langle 2;\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pccn$ (56)	$\langle 2;\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pccn$ (56)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pccn$ (56)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0);$ $5+(0,2u,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,2u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pccn$ (56)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/ncc$ (130); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Aema$ (64, $Cmce$); [2] $Bmeb$ (64, $Cmce$); [2] $Cccm$ (66); [2] $Ibam$ (72)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pccb$ (54, $Pcca$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pcca$ (54); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pmmn$ (59)

D_{2h}^{11} $P2/b2_1/c2_1/m$ No. 57 $Pbcm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $Pbc2_1$ (29, $Pca2_1$)	1; 2; 7; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P2cm$ (28, $Pma2$)	1; 4; 6; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,1/4,0$
[2] $Pb2_1m$ (26, $Pmc2_1$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $P22_12_1$ (18, $P2_12_12$)	1; 2; 3; 4	$\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/4,0$
[2] $P12_1/c1$ (14)	1; 3; 5; 7		
[2] $P2/b11$ (13, $P12/c1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $P112_1/m$ (11, $P112_1/m$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$			
$Pbnm$ (62, $Pnma$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{b},\mathbf{c},2\mathbf{a}$	
$Pbnm$ (62, $Pnma$)	$\langle 3;\ (2;\ 5)+(1,0,0)\rangle$	$\mathbf{b},\mathbf{c},2\mathbf{a}$	$1/2,0,0$
$Pbca$ (61)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pbca$ (61)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
$Pbna$ (60, $Pbcn$)	$\langle 5;\ (2;\ 3)+(1,0,0)\rangle$	$\mathbf{c},2\mathbf{a},\mathbf{b}$	
$Pbna$ (60, $Pbcn$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{c},2\mathbf{a},\mathbf{b}$	$1/2,0,0$
$Pbcm$ (57)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pbcm$ (57)	$\langle (2;\ 3;\ 5)+(1,0,0)\rangle$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pbcm$ (57)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pbcm$ (57)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pbcm$ (57)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pbcm$ (57)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pbcm$ (57)	$\langle (2;\ 5)+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pbcm$ (57)	$\langle (2;\ 5)+(0,4,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pbcm$ (57)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pbcm$ (57)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pbcm$ (57)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pbcm$ (57)	$\langle (2;\ 3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pbcm$ (57)	$\langle (2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pbcm$ (57)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmcm$ (63); [2] $Bbem$ (64, $Cmce$); [2] $Aemm$ (67, $Cmme$); [2] $Ibam$ (72)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pmcm$ (51, $Pmma$); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pbmm$ (51, $Pmma$)

$Pnnm$ No. 58 $P2_1/n2_1/n2/m$ D_{2h}^{12}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Pnn2$ (34)	1; 2; 7; 8		
[2] $Pn2_1m$ (31, $Pmn2_1$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,0,0$
[2] $P2_1nm$ (31, $Pmn2_1$)	1; 4; 6; 7	$-\mathbf{c},\mathbf{b},\mathbf{a}$	$0,1/4,0$
[2] $P2_12_12$ (18)	1; 2; 3; 4		$0,0,1/4$
[2] $P12_1/n1$ (14, $P12_1/c1$)	1; 3; 5; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}-\mathbf{c}$	
[2] $P2_1/n11$ (14, $P12_1/c1$)	1; 4; 5; 8	$-\mathbf{c},\mathbf{a},\mathbf{b}+\mathbf{c}$	
[2] $P112/m$ (10)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Pnnm$ (58)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pnnm$ (58)	$\langle (2;\ 5)+(2,0,0);\ 3+(3,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pnnm$ (58)	$\langle (2;\ 5)+(4,0,0);\ 3+(5,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pnnm$ (58)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pnnm$ (58)	$\langle (2;\ 5)+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pnnm$ (58)	$\langle (2;\ 5)+(0,4,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pnnm$ (58)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pnnm$ (58)	$\langle 2;\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pnnm$ (58)	$\langle 2;\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pnnm$ (58)	$\langle (2;\ 5)+(2u,0,0);\ 3+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pnnm$ (58)	$\langle (2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pnnm$ (58)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/mnc$ (128); [2] $P4_2/mnm$ (136)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Amam$ (63, $Cmcm$); [2] $Bbmm$ (63, $Cmcm$); [2] $Cccm$ (66); [2] $Immm$ (71)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pncm$ (53, $Pmna$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pcnm$ (53, $Pmna$); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pbam$ (55)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 59, pp. 171–173.

D_{2h}^{13} $P2_1/m2_1/m2/n$ No. 59 $Pmmn$

ORIGIN CHOICE 1, Origin at $mm2/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $Pm2_1n$ (31, $Pmn2_1$)	1; 3; 6; 8	$\mathbf{a},-\mathbf{c},\mathbf{b}$	
[2] $P2_1mn$ (31, $Pmn2_1$)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pmm2$ (25)	1; 2; 7; 8		
[2] $P2_12_12$ (18)	1; 2; 3; 4		
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $P12_1/m1$ (11)	1; 3; 5; 7		$1/4,1/4,0$
[2] $P2_1/m11$ (11, $P12_1/m1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$Pcmn$ (62, $Pnma$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{b},-\mathbf{a}$	$1/4,1/4,0$
$Pcmn$ (62, $Pnma$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{b},-\mathbf{a}$	$1/4,1/4,1/2$
$Pmcn$ (62, $Pnma$)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
$Pmcn$ (62, $Pnma$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,1/2$
$Pmmn$ (59)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$Pccn$ (56)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$1/4,1/4,0$
$Pccn$ (56)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$1/4,1/4,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pmmn$ (59)	$\langle 2+(2,0,0);\ (3;\ 5)+(3,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pmmn$ (59)	$\langle 2+(4,0,0);\ (3;\ 5)+(5,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pmmn$ (59)	$\langle 2+(0,2,0);\ 3+(0,1,0);\ 5+(0,3,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pmmn$ (59)	$\langle 2+(0,4,0);\ 3+(0,1,0);\ 5+(0,5,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pmmn$ (59)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pmmn$ (59)	$\langle 2+(2u,0,0);\ (3;\ 5)+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pmmn$ (59)	$\langle 2+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0);$ $5+(0,\frac{p}{2}-\frac{1}{2}+2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Amma* (63, *Cmcm*); [2] *Bmmb* (63, *Cmcm*); [2] *Cmmm* (65); [2] *Immm* (71)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pmmb* (51, *Pmma*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pmma* (51)

 (*Continued from the facing page*)

I Minimal *translationengleiche* supergroups

[2] $P4/nmm$ (129); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Amma* (63, *Cmcm*); [2] *Bmmb* (63, *Cmcm*); [2] *Cmmm* (65); [2] *Immm* (71)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Pmmb* (51, *Pmma*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pmma* (51)

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $2_1\,2_1\,n$, at $-\frac{1}{4},-\frac{1}{4},0$ from $mm2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y,z$

I Maximal *translationengleiche* subgroups

[2] $Pm2_1n$ (31, $Pmn2_1$)	1; 3; 6; 8	$\mathbf{a},-\mathbf{c},\mathbf{b}$	$1/4,1/4,0$
[2] $P2_1mn$ (31, $Pmn2_1$)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,1/4,0$
[2] $Pmm2$ (25)	1; 2; 7; 8		$1/4,1/4,0$
[2] $P2_12_12$ (18)	1; 2; 3; 4		$1/4,1/4,0$
[2] $P112/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P12_1/m1$ (11)	1; 3; 5; 7		
[2] $P2_1/m11$ (11, $P12_1/m1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$Pcmn$ (62, $Pnma$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{b},-\mathbf{a}$	
$Pcmn$ (62, $Pnma$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,0,1/2$
$Pmcn$ (62, $Pnma$)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	
$Pmcn$ (62, $Pnma$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/2$
$Pmmn$ (59)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$Pccn$ (56)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Pccn$ (56)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{a}'=3\mathbf{a}$			
$Pmmn$ (59)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pmmn$ (59)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pmmn$ (59)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pmmn$ (59)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pmmn$ (59)	$\langle 2+(0,3,0);\ 3+(0,1,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pmmn$ (59)	$\langle 2+(0,5,0);\ 3+(0,1,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pmmn$ (59)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Pmmn$ (59)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Pmmn$ (59)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0);$ $5+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Pmmn$ (59)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

(*Continued on the facing page*)

$Pbcn$ No. 60 $P2_1/b2/c2_1/n$ D_{2h}^{14}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
8 d 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
	(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P2_1cn$ (33, $Pna2_1$)	1; 4; 6; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,1/4,0$
[2] $Pb2n$ (30, $Pnc2$)	1; 3; 6; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $Pbc2_1$ (29, $Pca2_1$)	1; 2; 7; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $P2_122_1$ (18, $P2_12_12$)	1; 2; 3; 4	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,1/4,1/4$
[2] $P112_1/n$ (14, $P112_1/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $P2_1/b11$ (14, $P12_1/c1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $P12/c1$ (13)	1; 3; 5; 7		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Pbcn$ (60)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pbcn$ (60)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pbcn$ (60)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pbcn$ (60)	$\langle 3;\ 5;\ 2+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pbcn$ (60)	$\langle 3;\ 2+(0,3,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pbcn$ (60)	$\langle 3;\ 2+(0,5,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pbcn$ (60)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pbcn$ (60)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pbcn$ (60)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Pbcn$ (60)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Pbcn$ (60)	$\langle 3;\ 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 5+(0,2u,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Pbcn$ (60)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Cmcm$ (63); [2] $Aema$ (64, $Cmce$); [2] $Bbeb$ (68, $Ccce$); [2] $Ibam$ (72)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pbmn$ (53, $Pmna$); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pbcb$ (54, $Pcca$); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pmca$ (57, $Pbcm$)

D_{2h}^{15} $P2_1/b2_1/c2_1/a$ No. 61 $Pbca$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*c*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $Pbc2_1$ (29, $Pca2_1$)	1; 2; 7; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,0,0$
[2] $Pb2_1a$ (29, $Pca2_1$)	1; 3; 6; 8	$\mathbf{a},-\mathbf{c},\mathbf{b}$	$0,0,1/4$
[2] $P2_1ca$ (29, $Pca2_1$)	1; 4; 6; 7	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,1/4,0$
[2] $P2_12_12_1$ (19)	1; 2; 3; 4		
[2] $P112_1/a$ (14)	1; 2; 5; 6		
[2] $P12_1/c1$ (14)	1; 3; 5; 7		
[2] $P2_1/b11$ (14, $P12_1/c1$)	1; 4; 5; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
Pbca (61)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
Pbca (61)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
Pbca (61)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
Pbca (61)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
Pbca (61)	$\langle (2;\ 5)+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
Pbca (61)	$\langle (2;\ 5)+(0,4,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
Pbca (61)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
Pbca (61)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
Pbca (61)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
Pbca (61)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
Pbca (61)	$\langle (2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
Pbca (61)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[3] $Pa\bar{3}$ (205)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Aema* (64, *Cmce*); [2] *Bbem* (64, *Cmce*); [2] *Cmce* (64); [2] *Ibca* (73)

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ *Pbcm* (57); [2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ *Pmca* (57, *Pbcm*); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ *Pbma* (57, *Pbcm*)

$Pnma$ No. 62 $P2_1/n2_1/m2_1/a$ D_{2h}^{16}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

8 d 1

(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y+\frac{1}{2},\bar{z}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$

(5) $\bar{x},\bar{y},\bar{z}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Pn2_1a$ (33, $Pna2_1$)	1; 3; 6; 8	$\mathbf{a},-\mathbf{c},\mathbf{b}$	
[2] $Pnm2_1$ (31, $Pmn2_1$)	1; 2; 7; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $P2_1ma$ (26, $Pmc2_1$)	1; 4; 6; 7	$\mathbf{b},\mathbf{c},\mathbf{a}$	$0,1/4,1/4$
[2] $P2_12_12_1$ (19)	1; 2; 3; 4		$0,0,1/4$
[2] $P112_1/a$ (14)	1; 2; 5; 6		
[2] $P2_1/n11$ (14, $P12_1/c1$)	1; 4; 5; 8	$-\mathbf{b},\mathbf{a},\mathbf{b}+\mathbf{c}$	
[2] $P12_1/m1$ (11)	1; 3; 5; 7		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Pnma$ (62)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Pnma$ (62)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Pnma$ (62)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Pnma$ (62)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Pnma$ (62)	$\langle (2;\ 5)+(0,2,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Pnma$ (62)	$\langle (2;\ 5)+(0,4,0);\ 3+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Pnma$ (62)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Pnma$ (62)	$\langle 2+(0,0,1);\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Pnma$ (62)	$\langle 2+(0,0,1);\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Pnma$ (62)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Pnma$ (62)	$\langle (2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Pnma$ (62)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Amma$ (63, $Cmcm$); [2] $Bbmm$ (63, $Cmcm$); [2] $Ccme$ (64, $Cmce$); [2] $Imma$ (74)

- **Decreased unit cell**

[2] $\mathbf{b}'=\frac{1}{2}\mathbf{b}$ $Pcma$ (55, $Pbam$); [2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pbma$ (57, $Pbcm$); [2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $Pnmm$ (59, $Pmmn$)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 63, pp. 177–178.

D_{2h}^{17} $C2/m2/c2_1/m$ No. 63 $Cmcm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$
16 h 1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x,\bar{y},\bar{z}$
	(5) $\bar{x},\bar{y},\bar{z}$ (6) $x,y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$ (8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $C2cm$ (40, $Ama2$)	(1; 4; 6; 7)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] $Cm2m$ (38, $Amm2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	0,0,1/4
[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+		
[2] $C222_1$ (20)	(1; 2; 3; 4)+		
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		
[2] $C2/m11$ (12, $C12/m1$)	(1; 4; 5; 8)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112_1/m$ (11, $P112_1/m$)	(1; 2; 5; 6)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pbnm$ (62, $Pnma$)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pmcn$ (62, $Pnma$)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4,1/4,0
[2] $Pbcn$ (60)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $Pmnm$ (59, $Pmmn$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4,1/4,0
[2] $Pmnn$ (58, $Pnnm$)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pbcm$ (57)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$		1/4,1/4,0
[2] $Pbnn$ (52, $Pnna$)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	1/4,1/4,0
[2] $Pmcm$ (51, $Pmma$)	1; 2; 3; 4; 5; 6; 7; 8	$\mathbf{c},\mathbf{a},\mathbf{b}$	

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Cmcm$ (63)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Cmcm$ (63)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1,0,0
$Cmcm$ (63)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2,0,0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Cmcm$ (63)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Cmcm$ (63)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0,1,0
$Cmcm$ (63)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0,2,0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Cmcm$ (63)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Cmcm$ (63)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,1
$Cmcm$ (63)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Cmcm$ (63)	$\langle (2;\ 3;\ 5)+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Cmcm$ (63)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Cmcm$ (63)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[3] $P6_3/mcm$ (193); [3] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Fmmm* (69)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pmcm* (51, *Pmma*); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Cmmm* (65)

Cmce No. 64

(*Continued from the facing page*)

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] *Fmmm* (69)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Pmcm* (51, *Pmma*); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Cmme* (67)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 64, pp. 178–179.

D_{2h}^{18} $C\,2/m\,2/c\,2_1/e$ No. 64 $Cmce$

Former space-group symbol *Cmca*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			
16	*g*	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] *C2ce* (41, *Aea*2)	(1; 4; 6; 7)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] *Cm2e* (39, *Aem*2)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 0, 1/4
[2] $Cmc2_1$ (36)	(1; 2; 7; 8)+		0, 1/4, 0
[2] $C222_1$ (20)	(1; 2; 3; 4)+		1/4, 0, 0
[2] *C*12/*c*1 (15)	(1; 3; 5; 7)+		1/4, 1/4, 0
[2] $C112_1/e$ (14, $P112_1/a$)	(1; 2; 5; 6)+	$\mathbf{a},1/2(-\mathbf{a}+\mathbf{b}),\mathbf{c}$	
[2] *C*2/*m*11 (12, *C*12/*m*1)	(1; 4; 5; 8)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] *Pmnb* (62, *Pnma*)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 1/4, 0
[2] *Pbca* (61)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] *Pbna* (60, *Pbcn*)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 0
[2] *Pmca* (57, *Pbcm*)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	1/4, 1/4, 0
[2] *Pbnb* (56, *Pccn*)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] *Pmcb* (55, *Pbam*)	1; 2; 3; 4; 5; 6; 7; 8	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] *Pbcb* (54, *Pcca*)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 0
[2] *Pmna* (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$		

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
Cmce (64)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
Cmce (64)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
Cmce (64)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
Cmce (64)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
Cmce (64)	$\langle 2+(0,3,0);\ 3+(0,1,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
Cmce (64)	$\langle 2+(0,5,0);\ 3+(0,1,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
Cmce (64)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
Cmce (64)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
Cmce (64)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
Cmce (64)	$\langle (2;\ 3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
Cmce (64)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0);$ $5+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
Cmce (64)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

(*Continued on the facing page*)

Cmmm No. 65 $C2/m2/m2/m$ D_{2h}^{19}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			
16	*r*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] *Cm2m* (38, *Amm*2)	(1; 3; 6; 8)+	**c**, **a**, **b**	
[2] *C2mm* (38, *Amm*2)	(1; 4; 6; 7)+	**c**, **b**, −**a**	
[2] *Cmm*2 (35)	(1; 2; 7; 8)+		
[2] *C*222 (21)	(1; 2; 3; 4)+		
[2] $C12/m1$ (12)	(1; 3; 5; 7)+		
[2] $C2/m11$ (12, $C12/m1$)	(1; 4; 5; 8)+	−**b**, **a**, **c**	
[2] $C112/m$ (10, $P112/m$)	(1; 2; 5; 6)+	1/2(**a** − **b**), 1/2(**a** + **b**), **c**	

II Maximal *klassengleiche* subgroups

• Loss of centring translations

[2] *Pmmn* (59)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$		1/4, 1/4, 0
[2] *Pbam* (55)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] *Pbmn* (53, *Pmna*)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$	**b**, **c**, **a**	
[2] *Pman* (53, *Pmna*)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	**a**, −**c**, **b**	
[2] *Pmam* (51, *Pmma*)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	**a**, −**c**, **b**	1/4, 1/4, 0
[2] *Pbmm* (51, *Pmma*)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$	**b**, **c**, **a**	1/4, 1/4, 0
[2] *Pban* (50)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$		1/4, 1/4, 0
[2] *Pmmm* (47)	1; 2; 3; 4; 5; 6; 7; 8		

• Enlarged unit cell

[2] **c**′ = 2**c**			
Ibmm (74, *Imma*)	⟨3; 5; 2 + (0,0,1)⟩	**b**, 2**c**, **a**	
Ibmm (74, *Imma*)	⟨(2; 3; 5) + (0,0,1)⟩	**b**, 2**c**, **a**	0, 0, 1/2
Imam (74, *Imma*)	⟨5; (2; 3) + (0,0,1)⟩	**a**, −2**c**, **b**	
Imam (74, *Imma*)	⟨3; (2; 5) + (0,0,1)⟩	**a**, −2**c**, **b**	0, 0, 1/2
Ibam (72)	⟨2; 5; 3 + (0,0,1)⟩	**a**, **b**, 2**c**	
Ibam (72)	⟨2; 3; 5 + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
Immm (71)	⟨2; 3; 5⟩	**a**, **b**, 2**c**	
Immm (71)	⟨2; (3; 5) + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
Cccm (66)	⟨2; 5; 3 + (0,0,1)⟩	**a**, **b**, 2**c**	
Cccm (66)	⟨2; 3; 5 + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
Cmmm (65)	⟨2; 3; 5⟩	**a**, **b**, 2**c**	
Cmmm (65)	⟨2; (3; 5) + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
Ccmm (63, *Cmcm*)	⟨3; 5; 2 + (0,0,1)⟩	−**b**, **a**, 2**c**	
Ccmm (63, *Cmcm*)	⟨(2; 3; 5) + (0,0,1)⟩	−**b**, **a**, 2**c**	0, 0, 1/2
Cmcm (63)	⟨5; (2; 3) + (0,0,1)⟩	**a**, **b**, 2**c**	
Cmcm (63)	⟨3; (2; 5) + (0,0,1)⟩	**a**, **b**, 2**c**	0, 0, 1/2
[3] **a**′ = 3**a**			
Cmmm (65)	⟨2; 3; 5⟩	3**a**, **b**, **c**	
Cmmm (65)	⟨(2; 3; 5) + (2,0,0)⟩	3**a**, **b**, **c**	1, 0, 0
Cmmm (65)	⟨(2; 3; 5) + (4,0,0)⟩	3**a**, **b**, **c**	2, 0, 0
[3] **b**′ = 3**b**			
Cmmm (65)	⟨2; 3; 5⟩	**a**, 3**b**, **c**	
Cmmm (65)	⟨3; (2; 5) + (0,2,0)⟩	**a**, 3**b**, **c**	0, 1, 0
Cmmm (65)	⟨3; (2; 5) + (0,4,0)⟩	**a**, 3**b**, **c**	0, 2, 0
[3] **c**′ = 3**c**			
Cmmm (65)	⟨2; 3; 5⟩	**a**, **b**, 3**c**	
Cmmm (65)	⟨2; (3; 5) + (0,0,2)⟩	**a**, **b**, 3**c**	0, 0, 1
Cmmm (65)	⟨2; (3; 5) + (0,0,4)⟩	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
$Cmmm$ (65)	$\langle(2;\ 3;\ 5) + (2u, 0, 0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
$Cmmm$ (65)	$\langle 3;\ (2;\ 5) + (0, 2u, 0)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$Cmmm$ (65)	$\langle 2;\ (3;\ 5) + (0, 0, 2u)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4/mbm$ (127); [2] $P4_2/mcm$ (132); [2] $P4_2/mnm$ (136); [3] $P6/mmm$ (191)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmmm$ (69)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmmm$ (47)

(*Continued from the following page*) No. 66 $Cccm$

I Minimal *translationengleiche* supergroups

[2] $P4/mcc$ (124); [2] $P4/mnc$ (128); [2] $P4_2/mmc$ (131); [2] $P4_2/mbc$ (135); [3] $P6/mcc$ (192)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmmm$ (69)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pccm$ (49); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Cmmm$ (65)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 66, pp. 181–182.

$Cccm$ No. 66 $C2/c2/c2/m$ D_{2h}^{20}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$
16	m	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x,\bar{y},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x,y,\bar{z}$ (7) $x,\bar{y},z+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Cc2m$ (40, $Ama2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,0,1/4$
[2] $C2cm$ (40, $Ama2$)	(1; 4; 6; 7)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,0,1/4$
[2] $Ccc2$ (37)	(1; 2; 7; 8)+		
[2] $C222$ (21)	(1; 2; 3; 4)+		$0,0,1/4$
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		
[2] $C2/c11$ (15, $C12/c1$)	(1; 4; 5; 8)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $C112/m$ (10, $P112/m$)	(1; 2; 5; 6)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pnnm$ (58)	$1;\ 2;\ 5;\ 6;\ (3;\ 4;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$		
[2] $Pccn$ (56)	$1;\ 2;\ 7;\ 8;\ (3;\ 4;\ 5;\ 6)+(\frac{1}{2},\frac{1}{2},0)$		$1/4,1/4,0$
[2] $Pcnm$ (53, $Pmna$)	$1;\ 3;\ 6;\ 8;\ (2;\ 4;\ 5;\ 7)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$1/4,1/4,0$
[2] $Pncm$ (53, $Pmna$)	$1;\ 4;\ 6;\ 7;\ (2;\ 3;\ 5;\ 8)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$
[2] $Pncn$ (52, $Pnna$)	$1;\ 3;\ 5;\ 7;\ (2;\ 4;\ 6;\ 8)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $Pcnn$ (52, $Pnna$)	$1;\ 4;\ 5;\ 8;\ (2;\ 3;\ 6;\ 7)+(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] $Pccm$ (49)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $Pnnn$ (48)	$1;\ 2;\ 3;\ 4;\ (5;\ 6;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},0)$		$1/4,1/4,0$

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Cccm$ (66)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Cccm$ (66)	$\langle(2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Cccm$ (66)	$\langle(2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Cccm$ (66)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Cccm$ (66)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Cccm$ (66)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Cccm$ (66)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Cccm$ (66)	$\langle 2;\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Cccm$ (66)	$\langle 2;\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Cccm$ (66)	$\langle(2;\ 3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
[p] $\mathbf{b}'=p\mathbf{b}$			
$Cccm$ (66)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
[p] $\mathbf{c}'=p\mathbf{c}$			
$Cccm$ (66)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

(*Continued on the preceding page*)

D_{2h}^{21} $C2/m2/m2/e$ No. 67 $Cmme$

Former space-group symbol $Cmma$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$
16 *o* 1	(1) x,y,z (2) $\bar{x},\bar{y}+\frac{1}{2},z$ (3) $\bar{x},y+\frac{1}{2},\bar{z}$ (4) $x,\bar{y},\bar{z}$
	(5) $\bar{x},\bar{y},\bar{z}$ (6) $x,y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$ (8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $Cm2e$ (39, $Aem2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 0, 0
[2] $C2me$ (39, $Aem2$)	(1; 4; 6; 7)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] $Cmm2$ (35)	(1; 2; 7; 8)+		0, 1/4, 0
[2] $C222$ (21)	(1; 2; 3; 4)+		1/4, 0, 0
[2] $C112/e$ (13, $P112/a$)	(1; 2; 5; 6)+	$\mathbf{a},1/2(-\mathbf{a}+\mathbf{b}),\mathbf{c}$	
[2] $C12/m1$ (12)	(1; 3; 5; 7)+		1/4, 1/4, 0
[2] $C2/m11$ (12, $C12/m1$)	(1; 4; 5; 8)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

• Loss of centring translations

[2] $Pbma$ (57, $Pbcm$)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $Pmab$ (57, $Pbcm$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	1/4, 1/4, 0
[2] $Pbaa$ (54, $Pcca$)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	1/4, 1/4, 0
[2] $Pbab$ (54, $Pcca$)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{a},-\mathbf{c},\mathbf{b}$	
[2] $Pmmb$ (51, $Pmma$)	1; 2; 3; 4; 5; 6; 7; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Pmma$ (51)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$		1/4, 1/4, 0
[2] $Pmaa$ (49, $Pccm$)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pbmb$ (49, $Pccm$)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 0

• Enlarged unit cell

[2] $\mathbf{c}'=2\mathbf{c}$			
$Imma$ (74)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Imma$ (74)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	0, 0, 1/2
$Ibca$ (73)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Ibca$ (73)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	0, 0, 1/2
$Ibmb$ (72, $Ibam$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 1/2
$Ibmb$ (72, $Ibam$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 0
$Imaa$ (72, $Ibam$)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{b},2\mathbf{c},\mathbf{a}$	
$Imaa$ (72, $Ibam$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$\mathbf{b},2\mathbf{c},\mathbf{a}$	0, 0, 1/2
$Ccce$ (68)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	1/4, 1/4, 0
$Ccce$ (68)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	1/4, 1/4, 1/2
$Cmme$ (67)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Cmme$ (67)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	0, 0, 1/2
$Ccme$ (64, $Cmce$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a},2\mathbf{c}$	1/4, 1/4, 0
$Ccme$ (64, $Cmce$)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a},2\mathbf{c}$	1/4, 1/4, 1/2
$Cmce$ (64)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$Cmce$ (64)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	0, 0, 1/2
[3] $\mathbf{a}'=3\mathbf{a}$			
$Cmme$ (67)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Cmme$ (67)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$Cmme$ (67)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Cmme$ (67)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Cmme$ (67)	$\langle 2+(0,3,0);\ 3+(0,1,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$Cmme$ (67)	$\langle 2+(0,5,0);\ 3+(0,1,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Cmme$ (67)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Cmme$ (67)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$Cmme$ (67)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
Cmme (67)	$\langle (2;\ 3;\ 5) + (2u,0,0) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
Cmme (67)	$\langle 2 + (0, \frac{p}{2} - \frac{1}{2} + 2u, 0);\ 3 + (0, \frac{p}{2} - \frac{1}{2}, 0);$ $5 + (0, 2u, 0) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
Cmme (67)	$\langle 2;\ (3;\ 5) + (0,0,2u) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4/nmm$ (129); [2] $P4_2/nnm$ (134); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmmm$ (69)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pmmm$ (47)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 68, pp. 185–187.

D_{2h}^{22} $C2/c2/c2/e$ No. 68 $Ccce$

Former space-group symbol $Ccca$

ORIGIN CHOICE 1, Origin at 222 at $2/n2/n2$, at $0,\frac{1}{4},\frac{1}{4}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$

16	*i*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},y,\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Cc2e$ (41, $Aea2$)	(1; 3; 6; 8)+	**c**, **a**, **b**	
[2] $C2ce$ (41, $Aea2$)	(1; 4; 6; 7)+	**c**, **b**, −**a**	
[2] $Ccc2$ (37)	(1; 2; 7; 8)+		1/4, 1/4, 0
[2] $C222$ (21)	(1; 2; 3; 4)+		
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		0, 1/4, 1/4
[2] $C2/c11$ (15, $C12/c1$)	(1; 4; 5; 8)+	−**b**, **a**, **c**	1/4, 0, 1/4
[2] $C112/e$ (13, $P112/a$)	(1; 2; 5; 6)+	**a**, 1/2(−**a**+**b**), **c**	1/4, 0, 1/4

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pcnb$ (60, $Pbcn$)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	**a**, −**c**, **b**	0, 1/4, 1/4
[2] $Pnca$ (60, $Pbcn$)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$	**b**, **c**, **a**	1/4, 0, 1/4
[2] $Pcca$ (54)	1; 2; 3; 4; 5; 6; 7; 8		0, 1/4, 1/4
[2] $Pccb$ (54, $Pcca$)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$	−**b**, **a**, **c**	1/4, 0, 1/4
[2] $Pnnb$ (52, $Pnna$)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	−**b**, **a**, **c**	1/4, 0, 1/4
[2] $Pnna$ (52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$		0, 1/4, 1/4
[2] $Pncb$ (50, $Pban$)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$	**b**, **c**, **a**	
[2] $Pcna$ (50, $Pban$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	**c**, **a**, **b**	

- **Enlarged unit cell**

[3] **a**′ = 3**a**			
$Ccce$ (68)	⟨3; 5; 2 + (1,0,0)⟩	3**a**, **b**, **c**	
$Ccce$ (68)	⟨2 + (3,0,0); (3; 5) + (2,0,0)⟩	3**a**, **b**, **c**	1, 0, 0
$Ccce$ (68)	⟨2 + (5,0,0); (3; 5) + (4,0,0)⟩	3**a**, **b**, **c**	2, 0, 0
[3] **b**′ = 3**b**			
$Ccce$ (68)	⟨3; (2; 5) + (0,1,0)⟩	**a**, 3**b**, **c**	
$Ccce$ (68)	⟨3; (2; 5) + (0,3,0)⟩	**a**, 3**b**, **c**	0, 1, 0
$Ccce$ (68)	⟨3; (2; 5) + (0,5,0)⟩	**a**, 3**b**, **c**	0, 2, 0
[3] **c**′ = 3**c**			
$Ccce$ (68)	⟨2; 3; 5 + (0,0,1)⟩	**a**, **b**, 3**c**	
$Ccce$ (68)	⟨2; 3 + (0,0,2); 5 + (0,0,3)⟩	**a**, **b**, 3**c**	0, 0, 1
$Ccce$ (68)	⟨2; 3 + (0,0,4); 5 + (0,0,5)⟩	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] **a**′ = p**a**			
$Ccce$ (68)	⟨2 + $(\frac{p}{2}-\frac{1}{2}+2u,0,0)$; (3; 5) + $(2u,0,0)$⟩ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	p**a**, **b**, **c**	u, 0, 0
[p] **b**′ = p**b**			
$Ccce$ (68)	⟨3; (2; 5) + $(0,\frac{p}{2}-\frac{1}{2}+2u,0)$⟩ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	**a**, p**b**, **c**	0, u, 0
[p] **c**′ = p**c**			
$Ccce$ (68)	⟨2; 3 + $(0,0,2u)$; 5 + $(0,0,\frac{p}{2}-\frac{1}{2}+2u)$⟩ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	**a**, **b**, p**c**	0, 0, u

I Minimal *translationengleiche* supergroups

[2] $P4/nnc$ (126); [2] $P4/ncc$ (130); [2] $P4_2/nbc$ (133); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmmm$ (69)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pccm$ (49); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Cmme$ (67)

Ccce ORIGIN CHOICE 2 No. 68 (*Continued from the facing page*)

I Minimal *translationengleiche* supergroups

[2] $P4/nnc$ (126); [2] $P4/ncc$ (130); [2] $P4_2/nbc$ (133); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Fmmm$ (69)

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Pccm$ (49); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Cmme$ (67)

Former space-group symbol Cca

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $2/nca$, at $0,-\frac{1}{4},-\frac{1}{4}$ from 222

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			
16	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $Cc2e$ (41, $Aea2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,1/4,1/4$
[2] $C2ce$ (41, $Aea2$)	(1; 4; 6; 7)+	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$0,1/4,1/4$
[2] $Ccc2$ (37)	(1; 2; 7; 8)+		$1/4,0,1/4$
[2] $C222$ (21)	(1; 2; 3; 4)+		$0,1/4,1/4$
[2] $C12/c1$ (15)	(1; 3; 5; 7)+		
[2] $C2/c11$ (15, $C12/c1$)	(1; 4; 5; 8)+	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $C112/e$ (13, $P112/a$)	(1; 2; 5; 6)+	$\mathbf{a},1/2(-\mathbf{a}+\mathbf{b}),\mathbf{c}$	$1/4,1/4,0$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pcnb$ (60, $Pbcn$)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{a},-\mathbf{c},\mathbf{b}$	
[2] $Pnca$ (60, $Pbcn$)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,1/4,0$
[2] $Pcca$ (54)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $Pccb$ (54, $Pcca$)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $Pnnb$ (52, $Pnna$)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$
[2] $Pnna$ (52)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $Pncb$ (50, $Pban$)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pcna$ (50, $Pban$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/4,1/4,0$

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Ccce$ (68)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Ccce$ (68)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1,0,0$
$Ccce$ (68)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Ccce$ (68)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Ccce$ (68)	$\langle 3;\ (2;\ 5)+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,1,0$
$Ccce$ (68)	$\langle 3;\ (2;\ 5)+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$0,2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Ccce$ (68)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Ccce$ (68)	$\langle 2;\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$Ccce$ (68)	$\langle 2;\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Ccce$ (68)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Ccce$ (68)	$\langle 3;\ (2;\ 5)+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Ccce$ (68)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

(*Continued on the facing page*)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 69, pp. 188–189.

$Fmmm$ No. 69 $F2/m2/m2/m$ D_{2h}^{23}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
32	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $Fmm2$ (42)	(1; 2; 7; 8)+	
[2] $Fm2m$ (42, $Fmm2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$
[2] $F2mm$ (42, $Fmm2$)	(1; 4; 6; 7)+	$\mathbf{b},\mathbf{c},\mathbf{a}$
[2] $F222$ (22)	(1; 2; 3; 4)+	
[2] $F112/m$ (12, $A112/m$)	(1; 2; 5; 6)+	$1/2(\mathbf{a}-\mathbf{b}),\mathbf{b},\mathbf{c}$
[2] $F12/m1$ (12, $C12/m1$)	(1; 3; 5; 7)+	$\mathbf{a},\mathbf{b},1/2(-\mathbf{a}+\mathbf{c})$
[2] $F2/m11$ (12, $C12/m1$)	(1; 4; 5; 8)+	$-\mathbf{b},\mathbf{a},1/2(\mathbf{b}+\mathbf{c})$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Aeaa$ (68, $Ccce$)	1; 2; 3; 4; (1; 2; 3; 4) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	1/4, 1/4, 0
[2] $Bbeb$ (68, $Ccce$)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},0,\frac{1}{2})$; (5; 6; 7; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 0
[2] $Ccce$ (68)	1; 2; 3; 4; (1; 2; 3; 4) + $(\frac{1}{2},\frac{1}{2},0)$; (5; 6; 7; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (5; 6; 7; 8) + $(\frac{1}{2},0,\frac{1}{2})$		0, 1/4, 1/4
[2] $Cmme$ (67)	1; 2; 7; 8; (1; 2; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4; 5; 6) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4; 5; 6) + $(\frac{1}{2},0,\frac{1}{2})$		0, 1/4, 1/4
[2] $Bmem$ (67, $Cmme$)	1; 3; 6; 8; (1; 3; 6; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4; 5; 7) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 0
[2] $Aemm$ (67, $Cmme$)	1; 4; 6; 7; (1; 4; 6; 7) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3; 5; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	1/4, 0, 1/4
[2] $Cccm$ (66)	1; 2; 5; 6; (1; 2; 5; 6) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 4; 7; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2},0,\frac{1}{2})$		1/4, 1/4, 0
[2] $Bbmb$ (66, $Cccm$)	1; 3; 5; 7; (1; 3; 5; 7) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4; 6; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 0, 1/4
[2] $Amaa$ (66, $Cccm$)	1; 4; 5; 8; (1; 4; 5; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	0, 1/4, 1/4
[2] $Ammm$ (65, $Cmmm$)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + $(0,\frac{1}{2},\frac{1}{2})$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Bmmm$ (65, $Cmmm$)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + $(\frac{1}{2},0,\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $Cmmm$ (65)	1; 2; 3; 4; 5; 6; 7; 8; (1; 2; 3; 4; 5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$		
[2] $Aeam$ (64, $Cmce$)	1; 2; 5; 6; (1; 2; 5; 6) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	
[2] $Bbem$ (64, $Cmce$)	1; 2; 5; 6; (1; 2; 5; 6) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 4; 7; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $Aema$ (64, $Cmce$)	1; 3; 5; 7; (1; 3; 5; 7) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Ccme$ (64, $Cmce$)	1; 3; 5; 7; (1; 3; 5; 7) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 4; 6; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 4; 6; 8) + $(\frac{1}{2},0,\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Bmeb$ (64, $Cmce$)	1; 4; 5; 8; (1; 4; 5; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (2; 3; 6; 7) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},0)$	$\mathbf{a},-\mathbf{c},\mathbf{b}$	
[2] $Cmce$ (64)	1; 4; 5; 8; (1; 4; 5; 8) + $(\frac{1}{2},\frac{1}{2},0)$; (2; 3; 6; 7) + $(0,\frac{1}{2},\frac{1}{2})$; (2; 3; 6; 7) + $(\frac{1}{2},0,\frac{1}{2})$		

[2] *Amam* (63, *Cmcm*)	1; 3; 6; 8; (1; 3; 6; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4; 5; 7) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 4; 5; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$	$\mathbf{c}, \mathbf{b}, -\mathbf{a}$	$1/4, 1/4, 0$
[2] *Amma* (63, *Cmcm*)	1; 2; 7; 8; (1; 2; 7; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4; 5; 6) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$1/4, 0, 1/4$
[2] *Bmmb* (63, *Cmcm*)	1; 2; 7; 8; (1; 2; 7; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$; (3; 4; 5; 6) + $(0, \frac{1}{2}, \frac{1}{2})$; (3; 4; 5; 6) + $(\frac{1}{2}, \frac{1}{2}, 0)$	$\mathbf{a}, -\mathbf{c}, \mathbf{b}$	$0, 1/4, 1/4$
[2] *Bbmm* (63, *Cmcm*)	1; 4; 6; 7; (1; 4; 6; 7) + $(\frac{1}{2}, 0, \frac{1}{2})$; (2; 3; 5; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3; 5; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$1/4, 1/4, 0$
[2] *Cmcm* (63)	1; 3; 6; 8; (1; 3; 6; 8) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 4; 5; 7) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 4; 5; 7) + $(\frac{1}{2}, 0, \frac{1}{2})$		$0, 1/4, 1/4$
[2] *Ccmm* (63, *Cmcm*)	1; 4; 6; 7; (1; 4; 6; 7) + $(\frac{1}{2}, \frac{1}{2}, 0)$; (2; 3; 5; 8) + $(0, \frac{1}{2}, \frac{1}{2})$; (2; 3; 5; 8) + $(\frac{1}{2}, 0, \frac{1}{2})$	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$	$1/4, 0, 1/4$

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$

Fmmm (69)	$\langle 2;\ 3;\ 5 \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
Fmmm (69)	$\langle (2;\ 3;\ 5) + (2, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1, 0, 0$
Fmmm (69)	$\langle (2;\ 3;\ 5) + (4, 0, 0) \rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$2, 0, 0$

[3] $\mathbf{b}' = 3\mathbf{b}$

Fmmm (69)	$\langle 2;\ 3;\ 5 \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
Fmmm (69)	$\langle 3;\ (2;\ 5) + (0, 2, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 1, 0$
Fmmm (69)	$\langle 3;\ (2;\ 5) + (0, 4, 0) \rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 2, 0$

[3] $\mathbf{c}' = 3\mathbf{c}$

Fmmm (69)	$\langle 2;\ 3;\ 5 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
Fmmm (69)	$\langle 2;\ (3;\ 5) + (0, 0, 2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 1$
Fmmm (69)	$\langle 2;\ (3;\ 5) + (0, 0, 4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$0, 0, 2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = p\mathbf{a}$

Fmmm (69)	$\langle (2;\ 3;\ 5) + (2u, 0, 0) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$u, 0, 0$

[p] $\mathbf{b}' = p\mathbf{b}$

Fmmm (69)	$\langle 3;\ (2;\ 5) + (0, 2u, 0) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$0, u, 0$

[p] $\mathbf{c}' = p\mathbf{c}$

Fmmm (69)	$\langle 2;\ (3;\ 5) + (0, 0, 2u) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$

I Minimal *translationengleiche* supergroups

[2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $Fm\bar{3}$ (202)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Pmmm* (47)

$Fddd$ No. 70 $F2/d2/d2/d$ D_{2h}^{24}

ORIGIN CHOICE 1, Origin at 222, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$			
32 h 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
	(5) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(6) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(7) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(8) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $Fdd2$ (43)	(1; 2; 7; 8)+		
[2] $Fd2d$ (43, $Fdd2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $F2dd$ (43, $Fdd2$)	(1; 4; 6; 7)+	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $F222$ (22)	(1; 2; 3; 4)+		
[2] $F112/d$ (15, $A112/a$)	(1; 2; 5; 6)+	$1/2(\mathbf{a}-\mathbf{b}),\mathbf{b},\mathbf{c}$	$1/8,3/8,3/8$
[2] $F12/d1$ (15, $C12/c1$)	(1; 3; 5; 7)+	$-\mathbf{c},\mathbf{b},1/2(\mathbf{a}+\mathbf{c})$	$1/8,1/8,1/8$
[2] $F2/d11$ (15, $C12/c1$)	(1; 4; 5; 8)+	$-\mathbf{b},\mathbf{a},1/2(\mathbf{b}+\mathbf{c})$	$1/8,1/8,1/8$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(1,\frac{1}{2},\frac{1}{2})\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$1/4,1/4,1/4$
$Fddd$ (70)	$\langle 2+(\frac{5}{2},\frac{1}{2},0);\ 3+(\frac{5}{2},0,\frac{1}{2});\ 5+(3,\frac{1}{2},\frac{1}{2})\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$5/4,1/4,1/4$
$Fddd$ (70)	$\langle 2+(\frac{9}{2},\frac{1}{2},0);\ 3+(\frac{9}{2},0,\frac{1}{2});\ 5+(5,\frac{1}{2},\frac{1}{2})\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$9/4,1/4,1/4$
[3] $\mathbf{b}'=3\mathbf{b}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(\frac{1}{2},1,\frac{1}{2})\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$1/4,1/4,1/4$
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{5}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(\frac{1}{2},3,\frac{1}{2})\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$1/4,5/4,1/4$
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{9}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(\frac{1}{2},5,\frac{1}{2})\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$1/4,9/4,1/4$
[3] $\mathbf{c}'=3\mathbf{c}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(\frac{1}{2},\frac{1}{2},1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/4,1/4,1/4$
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{5}{2});\ 5+(\frac{1}{2},\frac{1}{2},3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/4,1/4,5/4$
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{9}{2});\ 5+(\frac{1}{2},\frac{1}{2},5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/4,1/4,9/4$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=p\mathbf{a}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2}+2u,\frac{1}{2},0);\ 3+(\frac{1}{2}+2u,0,\frac{1}{2});$ $5+(\frac{p}{4}+\frac{1}{4}+2u,\frac{1}{2},\frac{1}{2})\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$1/4+u,1/4,1/4$
$Fddd$ (70)	$\langle (2;\ 3)+(2u,0,0);\ 5+(\frac{p}{4}-\frac{1}{4}+2u,0,0)\rangle$ $p>4;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}'=p\mathbf{b}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2}+2u,0);\ 3+(\frac{1}{2},0,\frac{1}{2});$ $5+(\frac{1}{2},\frac{p}{4}+\frac{1}{4}+2u,\frac{1}{2})\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$1/4,1/4+u,1/4$
$Fddd$ (70)	$\langle 3;\ 2+(0,2u,0);\ 5+(0,\frac{p}{4}-\frac{1}{4}+2u,0)\rangle$ $p>4;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2}+2u);$ $5+(\frac{1}{2},\frac{1}{2},\frac{p}{4}+\frac{1}{4}+2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/4,1/4,1/4+u$
$Fddd$ (70)	$\langle 2;\ 3+(0,0,2u);\ 5+(0,0,\frac{p}{4}-\frac{1}{4}+2u)\rangle$ $p>4;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Pnnn* (48)

(*Continued from the following page*)

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $Fd\bar{3}$ (203)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Pnnn* (48)

$Fddd$ No. 70 $F2/d2/d2/d$ D_{2h}^{24}

ORIGIN CHOICE 2, Origin at $\bar{1}$ at ddd, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from 222

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$
32	h	1	(1) x,y,z (2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},z$ (3) $\bar{x}+\frac{3}{4},y,\bar{z}+\frac{3}{4}$ (4) $x,\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}$ (7) $x+\frac{1}{4},\bar{y},z+\frac{1}{4}$ (8) $\bar{x},y+\frac{1}{4},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $Fdd2$ (43)	(1; 2; 7; 8)+		3/8, 3/8, 0
[2] $Fd2d$ (43, $Fdd2$)	(1; 3; 6; 8)+	**c**, **a**, **b**	3/8, 0, 3/8
[2] $F2dd$ (43, $Fdd2$)	(1; 4; 6; 7)+	**b**, **c**, **a**	0, 3/8, 3/8
[2] $F222$ (22)	(1; 2; 3; 4)+		1/8, 1/8, 1/8
[2] $F112/d$ (15, $A112/a$)	(1; 2; 5; 6)+	1/2(**a** − **b**), **b**, **c**	0, 1/4, 1/4
[2] $F12/d1$ (15, $C12/c1$)	(1; 3; 5; 7)+	−**c**, **b**, 1/2(**a** + **c**)	
[2] $F2/d11$ (15, $C12/c1$)	(1; 4; 5; 8)+	−**b**, **a**, 1/2(**b** + **c**)	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Fddd$ (70)	$\langle 2+(\frac{3}{2},\frac{1}{2},0);\ 3+(\frac{3}{2},0,\frac{1}{2});\ 5+(0,\frac{1}{2},\frac{1}{2})\rangle$	3**a**, **b**, **c**	0, 1/4, 1/4
$Fddd$ (70)	$\langle 2+(\frac{7}{2},\frac{1}{2},0);\ 3+(\frac{7}{2},0,\frac{1}{2});\ 5+(2,\frac{1}{2},\frac{1}{2})\rangle$	3**a**, **b**, **c**	1, 1/4, 1/4
$Fddd$ (70)	$\langle 2+(\frac{11}{2},\frac{1}{2},0);\ 3+(\frac{11}{2},0,\frac{1}{2});\ 5+(4,\frac{1}{2},\frac{1}{2})\rangle$	3**a**, **b**, **c**	2, 1/4, 1/4
[3] $\mathbf{b}'=3\mathbf{b}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{3}{2},0);\ (3;\ 5)+(\frac{1}{2},0,\frac{1}{2})\rangle$	**a**, 3**b**, **c**	1/4, 0, 1/4
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{7}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(\frac{1}{2},2,\frac{1}{2})\rangle$	**a**, 3**b**, **c**	1/4, 1, 1/4
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{11}{2},0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(\frac{1}{2},4,\frac{1}{2})\rangle$	**a**, 3**b**, **c**	1/4, 2, 1/4
[3] $\mathbf{c}'=3\mathbf{c}$			
$Fddd$ (70)	$\langle (2;\ 5)+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{3}{2})\rangle$	**a**, **b**, 3**c**	1/4, 1/4, 0
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{7}{2});\ 5+(\frac{1}{2},\frac{1}{2},2)\rangle$	**a**, **b**, 3**c**	1/4, 1/4, 1
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{11}{2});\ 5+(\frac{1}{2},\frac{1}{2},4)\rangle$	**a**, **b**, 3**c**	1/4, 1/4, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Fddd$ (70)	$\langle 2+(\frac{3p}{4}-\frac{3}{4}+2u,\frac{1}{2},0);\ 3+(\frac{3p}{4}-\frac{3}{4}+2u,0,\frac{1}{2});\ 5+(2u,\frac{1}{2},\frac{1}{2})\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	p**a**, **b**, **c**	u, 1/4, 1/4
$Fddd$ (70)	$\langle (2;\ 3)+(\frac{3p}{4}-\frac{3}{4}+2u,0,0);\ 5+(2u,0,0)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	p**a**, **b**, **c**	u, 0, 0
[p] $\mathbf{b}'=p\mathbf{b}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{3p}{4}-\frac{3}{4}+2u,0);\ 3+(\frac{1}{2},0,\frac{1}{2});\ 5+(\frac{1}{2},2u,\frac{1}{2})\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	**a**, p**b**, **c**	1/4, u, 1/4
$Fddd$ (70)	$\langle 3;\ 2+(0,\frac{3p}{4}-\frac{3}{4}+2u,0);\ 5+(0,2u,0)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	**a**, p**b**, **c**	0, u, 0
[p] $\mathbf{c}'=p\mathbf{c}$			
$Fddd$ (70)	$\langle 2+(\frac{1}{2},\frac{1}{2},0);\ 3+(\frac{1}{2},0,\frac{3p}{4}-\frac{3}{4}+2u);\ 5+(\frac{1}{2},\frac{1}{2},2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	**a**, **b**, p**c**	1/4, 1/4, u
$Fddd$ (70)	$\langle 2;\ 3+(0,0,\frac{3p}{4}-\frac{3}{4}+2u);\ 5+(0,0,2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	**a**, **b**, p**c**	0, 0, u

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D_{2h}^{25} $I2/m2/m2/m$ No. 71 $Immm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	o	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $Imm2$ (44)	(1; 2; 7; 8)+		
[2] $Im2m$ (44, $Imm2$)	(1; 3; 6; 8)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $I2mm$ (44, $Imm2$)	(1; 4; 6; 7)+	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $I222$ (23)	(1; 2; 3; 4)+		
[2] $I112/m$ (12, $A112/m$)	(1; 2; 5; 6)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[2] $I12/m1$ (12, $C12/m1$)	(1; 3; 5; 7)+	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	
[2] $I2/m11$ (12, $C12/m1$)	(1; 4; 5; 8)+	$-\mathbf{b}+\mathbf{c},\mathbf{a},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pmmn$ (59)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $Pmnm$ (59, $Pmmn$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/4, 1/4, 1/4
[2] $Pnmm$ (59, $Pmmn$)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{b},\mathbf{c},\mathbf{a}$	1/4, 1/4, 1/4
[2] $Pnnm$ (58)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $Pnmn$ (58, $Pnnm$)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[2] $Pmnn$ (58, $Pnnm$)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Pnnn$ (48)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $Pmmm$ (47)	1; 2; 3; 4; 5; 6; 7; 8		

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$			
$Immm$ (71)	$\langle 2; 3; 5 \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Immm$ (71)	$\langle (2; 3; 5) + (2,0,0) \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$Immm$ (71)	$\langle (2; 3; 5) + (4,0,0) \rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}' = 3\mathbf{b}$			
$Immm$ (71)	$\langle 2; 3; 5 \rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Immm$ (71)	$\langle 3; (2; 5) + (0,2,0) \rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$Immm$ (71)	$\langle 3; (2; 5) + (0,4,0) \rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}' = 3\mathbf{c}$			
$Immm$ (71)	$\langle 2; 3; 5 \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Immm$ (71)	$\langle 2; (3; 5) + (0,0,2) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$Immm$ (71)	$\langle 2; (3; 5) + (0,0,4) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}' = p\mathbf{a}$			
$Immm$ (71)	$\langle (2; 3; 5) + (2u,0,0) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$u,0,0$
$[p]$ $\mathbf{b}' = p\mathbf{b}$			
$Immm$ (71)	$\langle 3; (2; 5) + (0,2u,0) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$0,u,0$
$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$Immm$ (71)	$\langle 2; (3; 5) + (0,0,2u) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

I Minimal *translationengleiche* supergroups

[2] $I4/mmm$ (139); [3] $Im\bar{3}$ (204)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $Ammm$ (65, $Cmmm$); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ $Bmmm$ (65, $Cmmm$); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Cmmm$ (65)

$Ibam$ No. 72 $I2/b2/a2/m$ D_{2h}^{26}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $Ib2m$ (46, $Ima2$)	(1; 3; 6; 8)+	**c**, **a**, **b**	0, 0, 1/4
[2] $I2am$ (46, $Ima2$)	(1; 4; 6; 7)+	**c**, **b**, −**a**	0, 0, 1/4
[2] $Iba2$ (45)	(1; 2; 7; 8)+		
[2] $I222$ (23)	(1; 2; 3; 4)+		0, 0, 1/4
[2] $I12/a1$ (15, $C12/c1$)	(1; 3; 5; 7)+	**a** − **c**, **b**, **c**	
[2] $I2/b11$ (15, $C12/c1$)	(1; 4; 5; 8)+	−**b** − **c**, **a**, **c**	
[2] $I112/m$ (12, $A112/m$)	(1; 2; 5; 6)+	**b**, −**a** − **b**, **c**	

II Maximal *klassengleiche* subgroups

• **Loss of centring translations**

[2] $Pcan$ (60, $Pbcn$)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	−**b**, **a**, **c**	
[2] $Pbcn$ (60)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $Pbcm$ (57)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $Pcam$ (57, $Pbcm$)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	−**b**, **a**, **c**	1/4, 1/4, 1/4
[2] $Pccn$ (56)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $Pbam$ (55)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $Pban$ (50)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $Pccm$ (49)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		

• **Enlarged unit cell**

[3] **a**′ = 3**a**			
$Ibam$ (72)	⟨2; 5; 3 + (1,0,0)⟩	3**a**, **b**, **c**	
$Ibam$ (72)	⟨(2; 5) + (2,0,0); 3 + (3,0,0)⟩	3**a**, **b**, **c**	1, 0, 0
$Ibam$ (72)	⟨(2; 5) + (4,0,0); 3 + (5,0,0)⟩	3**a**, **b**, **c**	2, 0, 0
[3] **b**′ = 3**b**			
$Ibam$ (72)	⟨2; 5; 3 + (0,1,0)⟩	**a**, 3**b**, **c**	
$Ibam$ (72)	⟨(2; 5) + (0,2,0); 3 + (0,1,0)⟩	**a**, 3**b**, **c**	0, 1, 0
$Ibam$ (72)	⟨(2; 5) + (0,4,0); 3 + (0,1,0)⟩	**a**, 3**b**, **c**	0, 2, 0
[3] **c**′ = 3**c**			
$Ibam$ (72)	⟨2; 3; 5⟩	**a**, **b**, 3**c**	
$Ibam$ (72)	⟨2; (3; 5) + (0,0,2)⟩	**a**, **b**, 3**c**	0, 0, 1
$Ibam$ (72)	⟨2; (3; 5) + (0,0,4)⟩	**a**, **b**, 3**c**	0, 0, 2

• **Series of maximal isomorphic subgroups**

[p] **a**′ = p**a**			
$Ibam$ (72)	⟨(2; 5) + $(2u,0,0)$; 3 + $(\frac{p}{2}-\frac{1}{2}+2u,0,0)$⟩ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	p**a**, **b**, **c**	u, 0, 0
[p] **b**′ = p**b**			
$Ibam$ (72)	⟨(2; 5) + $(0,2u,0)$; 3 + $(0,\frac{p}{2}-\frac{1}{2},0)$⟩ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	**a**, p**b**, **c**	0, u, 0
[p] **c**′ = p**c**			
$Ibam$ (72)	⟨2; (3; 5) + $(0,0,2u)$⟩ $p>2$; $0 \le u < p$ p conjugate subgroups for the prime p	**a**, **b**, p**c**	0, 0, u

I Minimal *translationengleiche* supergroups

[2] $I4/mcm$ (140)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations** none

• **Decreased unit cell**

[2] **c**′ = $\frac{1}{2}$**c** $Cmmm$ (65); [2] **a**′ = $\frac{1}{2}$**a** $Aemm$ (67, $Cmme$); [2] **b**′ = $\frac{1}{2}$**b** $Bmem$ (67, $Cmme$)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 73, pp. 195–196.

D_{2h}^{27} $I2_1/b2_1/c2_1/a$ No. 73 *Ibca*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
16	*f*	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $Ibc2$ (45, $Iba2$)	(1; 2; 7; 8)+		0, 1/4, 0
[2] $Ib2a$ (45, $Iba2$)	(1; 3; 6; 8)+	**c**, **a**, **b**	1/4, 0, 0
[2] $I2ca$ (45, $Iba2$)	(1; 4; 6; 7)+	**b**, **c**, **a**	0, 0, 1/4
[2] $I2_12_12_1$ (24)	(1; 2; 3; 4)+		
[2] $I112/a$ (15, $A112/a$)	(1; 2; 5; 6)+	**b**, −**a** − **b**, **c**	
[2] $I12/c1$ (15, $C12/c1$)	(1; 3; 5; 7)+	−**a** − **c**, **b**, **a**	
[2] $I2/b11$ (15, $C12/c1$)	(1; 4; 5; 8)+	−**b** − **c**, **a**, **c**	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pbca$ (61)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $Pcab$ (61, $Pbca$)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	−**b**, **a**, **c**	1/4, 1/4, 1/4
[2] $Pcaa$ (54, $Pcca$)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	**c**, **b**, −**a**	
[2] $Pccb$ (54, $Pcca$)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	−**b**, **a**, **c**	
[2] $Pbab$ (54, $Pcca$)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	**a**, −**c**, **b**	
[2] $Pbcb$ (54, $Pcca$)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	**c**, **a**, **b**	1/4, 1/4, 1/4
[2] $Pbaa$ (54, $Pcca$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	**b**, **c**, **a**	1/4, 1/4, 1/4
[2] $Pcca$ (54)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4

- **Enlarged unit cell**

[3] **a**′ = 3**a**			
$Ibca$ (73)	$\langle 3;\ 5;\ 2+(1,0,0)\rangle$	3**a**, **b**, **c**	
$Ibca$ (73)	$\langle 2+(3,0,0);\ (3;\ 5)+(2,0,0)\rangle$	3**a**, **b**, **c**	1, 0, 0
$Ibca$ (73)	$\langle 2+(5,0,0);\ (3;\ 5)+(4,0,0)\rangle$	3**a**, **b**, **c**	2, 0, 0
[3] **b**′ = 3**b**			
$Ibca$ (73)	$\langle 2;\ 5;\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	
$Ibca$ (73)	$\langle (2;\ 5)+(0,2,0);\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	0, 1, 0
$Ibca$ (73)	$\langle (2;\ 5)+(0,4,0);\ 3+(0,1,0)\rangle$	**a**, 3**b**, **c**	0, 2, 0
[3] **c**′ = 3**c**			
$Ibca$ (73)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	**a**, **b**, 3**c**	
$Ibca$ (73)	$\langle 2+(0,0,1);\ 3+(0,0,3);\ 5+(0,0,2)\rangle$	**a**, **b**, 3**c**	0, 0, 1
$Ibca$ (73)	$\langle 2+(0,0,1);\ 3+(0,0,5);\ 5+(0,0,4)\rangle$	**a**, **b**, 3**c**	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] **a**′ = p**a**			
$Ibca$ (73)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ (3;\ 5)+(2u,0,0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	p**a**, **b**, **c**	u, 0, 0
[p] **b**′ = p**b**			
$Ibca$ (73)	$\langle (2;\ 5)+(0,2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	**a**, p**b**, **c**	0, u, 0
[p] **c**′ = p**c**			
$Ibca$ (73)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $5+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	**a**, **b**, p**c**	0, 0, u

I Minimal *translationengleiche* supergroups

[2] $I4_1/acd$ (142); [2] $Ia\bar{3}$ (206)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Aemm* (67, *Cmme*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Bmem* (67, *Cmme*); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Cmme* (67)

$Imma$ No. 74

(*Continued from the facing page*)

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$ *Ammm* (65, *Cmmm*); [2] $\mathbf{b}' = \frac{1}{2}\mathbf{b}$ *Bmmm* (65, *Cmmm*); [2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ *Cmme* (67)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 74, pp. 196–197.

D_{2h}^{28} $I2_1/m2_1/m2_1/a$ No. 74 $Imma$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
16	j	1	(1) x,y,z (2) $\bar{x},\bar{y}+\frac{1}{2},z$ (3) $\bar{x},y+\frac{1}{2},\bar{z}$ (4) $x,\bar{y},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x,y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$ (8) $\bar{x},y,z$

I Maximal *translationengleiche* subgroups

[2] $Im2b$ (46, $Ima2$)	(1; 3; 6; 8)+	$-\mathbf{a},\mathbf{c},\mathbf{b}$	1/4, 0, 1/4
[2] $I2mb$ (46, $Ima2$)	(1; 4; 6; 7)+	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[2] $Imm2$ (44)	(1; 2; 7; 8)+		0, 1/4, 0
[2] $I2_12_12_1$ (24)	(1; 2; 3; 4)+		0, 0, 1/4
[2] $I112/b$ (15, $A112/a$)	(1; 2; 5; 6)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[2] $I12/m1$ (12, $C12/m1$)	(1; 3; 5; 7)+	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	1/4, 1/4, 1/4
[2] $I2/m11$ (12, $C12/m1$)	(1; 4; 5; 8)+	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pnma$ (62)	1; 3; 5; 7; (2; 4; 6; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $Pmnb$ (62, $Pnma$)	1; 3; 6; 8; (2; 4; 5; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 1/4, 1/4
[2] $Pnmb$ (53, $Pmna$)	1; 4; 6; 7; (2; 3; 5; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	1/4, 1/4, 1/4
[2] $Pmna$ (53)	1; 4; 5; 8; (2; 3; 6; 7) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $Pnna$ (52)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $Pnnb$ (52, $Pnna$)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[2] $Pmma$ (51)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $Pmmb$ (51, $Pmma$)	1; 2; 3; 4; 5; 6; 7; 8	$-\mathbf{b},\mathbf{a},\mathbf{c}$	

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$			
$Imma$ (74)	$\langle 2;\ 3;\ 5\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	
$Imma$ (74)	$\langle (2;\ 3;\ 5)+(2,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	1, 0, 0
$Imma$ (74)	$\langle (2;\ 3;\ 5)+(4,0,0)\rangle$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	2, 0, 0
[3] $\mathbf{b}'=3\mathbf{b}$			
$Imma$ (74)	$\langle 5;\ (2;\ 3)+(0,1,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	
$Imma$ (74)	$\langle 2+(0,3,0);\ 3+(0,1,0);\ 5+(0,2,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 1, 0
$Imma$ (74)	$\langle 2+(0,5,0);\ 3+(0,1,0);\ 5+(0,4,0)\rangle$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	0, 2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$Imma$ (74)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$Imma$ (74)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$Imma$ (74)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=p\mathbf{a}$			
$Imma$ (74)	$\langle (2;\ 3;\ 5)+(2u,0,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$p\mathbf{a},\mathbf{b},\mathbf{c}$	u, 0, 0
[p] $\mathbf{b}'=p\mathbf{b}$			
$Imma$ (74)	$\langle 2+(0,\frac{p}{2}-\frac{1}{2}+2u,0);\ 3+(0,\frac{p}{2}-\frac{1}{2},0);$ $5+(0,2u,0)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},p\mathbf{b},\mathbf{c}$	0, u, 0
[p] $\mathbf{c}'=p\mathbf{c}$			
$Imma$ (74)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	0, 0, u

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$P4$ No. 75 $P4$ C_4^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	d	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$

I Maximal *translationengleiche* subgroups

[2] $P2$ (3, $P112$)	1; 2

II Maximal *klassengleiche* subgroups

● **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2$ (77)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4$ (75)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$C4$ (75, $P4$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4$ (75, $P4$)	$\langle 2+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$F4$ (79, $I4$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4$ (79, $I4$)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4$ (75)	$\langle 2;\ 3\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

● **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4$ (75)	$\langle 2;\ 3\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P4$ (75)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p = q^2+r^2$] $\mathbf{a}' = q\mathbf{a}-r\mathbf{b},\ \mathbf{b}' = r\mathbf{a}+q\mathbf{b}$			
$P4$ (75)	$\langle 2+(2u,0,0);\ 3+(u,-u,0)\rangle$ $q>0;\ r>0;\ p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4/m$ (83); [2] $P4/n$ (85); [2] $P422$ (89); [2] $P42_12$ (90); [2] $P4mm$ (99); [2] $P4bm$ (100); [2] $P4cc$ (103); [2] $P4nc$ (104)

II Minimal non-isomorphic *klassengleiche* supergroups

● **Additional centring translations**

[2] $I4$ (79)

● **Decreased unit cell** none

C_4^2 $P4_1$ No. 76 $P4_1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	*a*	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{y},x,z+\frac{1}{4}$ (4) $y,\bar{x},z+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $P2_1$ (4, $P112_1$) 1; 2

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
$C4_1$ (76, $P4_1$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_1$ (76, $P4_1$)	$\langle 2+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_3$ (78)	$\langle 2+(0,0,1);\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_3$ (78)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{3p}{4}-\frac{1}{4})\rangle$ $p>2$; $p\equiv 3 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P4_1$ (76)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4})\rangle$ $p>4$; $p\equiv 1 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P4_1$ (76)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$P4_1$ (76)	$\langle 2+(2u,0,0);\ 3+(u,-u,0)\rangle$ $q>0$; $r>0$; $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4_122$ (91); [2] $P4_12_12$ (92)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4_1$ (80)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4_2$ (77)

$P4_2$ No. 77 $P4_2$ C_4^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	d	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z+\frac{1}{2}$ (4) $y,\bar{x},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P2$ (3, $P112$)	1; 2

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_3$ (78)	$\langle(2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_1$ (76)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$C4_2$ (77, $P4_2$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2$ (77, $P4_2$)	$\langle 2+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$F4_1$ (80, $I4_1$)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$F4_1$ (80, $I4_1$)	$\langle(2;\ 3)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,0,0$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4_2$ (77)	$\langle 2;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4_2$ (77)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P4_2$ (77)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2$] $\mathbf{a}' = q\mathbf{a}-r\mathbf{b},\ \mathbf{b}' = r\mathbf{a}+q\mathbf{b}$			
$P4_2$ (77)	$\langle 2+(2u,0,0);\ 3+(u,-u,0)\rangle$ $q>0;\ r>0;\ p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/m$ (84); [2] $P4_2/n$ (86); [2] $P4_222$ (93); [2] $P4_22_12$ (94); [2] $P4_2cm$ (101); [2] $P4_2nm$ (102); [2] $P4_2mc$ (105); [2] $P4_2bc$ (106)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4$ (79)

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P4$ (75)

C_4^4 $P4_3$ No. 78 $P4_3$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	a	1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$ (3) $\bar{y},x,z+\frac{3}{4}$ (4) $y,\bar{x},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $P2_1$ (4, $P112_1$) 1; 2

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4_3$ (78, $P4_3$)	$\langle 2;\ 3\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_3$ (78, $P4_3$)	$\langle 2+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_1$ (76)	$\langle 3;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P4_3$ (78)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{3p}{4}-\frac{3}{4})\rangle$ $p>4;\ p\equiv 1 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P4_1$ (76)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{3}{4})\rangle$ $p>2;\ p\equiv 3 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_3$ (78)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p>2$ p^2 conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$P4_3$ (78)	$\langle 2+(2u,0,0);\ 3+(u,-u,0)\rangle$ $q>0;\ r>0;\ p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4_322$ (95); [2] $P4_32_12$ (96)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4_1$ (80)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4_2$ (77)

$I4$ No. 79 $I4$ C_4^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8	c	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$

I Maximal *translationengleiche* subgroups

[2] $I2$ (5, $A112$) (1; 2)+ $\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2$ (77) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ 1/2, 0, 0
[2] $P4$ (75) 1; 2; 3; 4

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$
$I4$ (79) $\langle 2;\ 3\rangle$ $\mathbf{a},\mathbf{b},3\mathbf{c}$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$
$I4$ (79) $\langle 2;\ 3\rangle$ $\mathbf{a},\mathbf{b},p\mathbf{c}$
$p > 2$
no conjugate subgroups

[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$
$I4$ (79) $\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p\mathbf{a},p\mathbf{b},\mathbf{c}$ $u,v,0$
$p > 2;\ 0 \le u < p;\ 0 \le v < p$
p^2 conjugate subgroups for prime $p \equiv 3 \pmod 4$

[$p = q^2 + r^2$] $\mathbf{a}' = q\mathbf{a} - r\mathbf{b},\ \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$
$I4$ (79) $\langle 2+(2u,0,0);\ 3+(u,-u,0)\rangle$ $q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$ $u,0,0$
$q > 0;\ r > 0;\ p > 4;\ 0 \le u < p$
p conjugate subgroups for prime $p \equiv 1 \pmod 4$

I Minimal *translationengleiche* supergroups

[2] $I4/m$ (87); [2] $I422$ (97); [2] $I4mm$ (107); [2] $I4cm$ (108)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4$ (75, $P4$)

C_4^6 $I4_1$ No. 80 $I4_1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8	b	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$ (4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $I2$ (5, $A112$)	(1; 2)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_3$ (78)	1; 2; $(3;\ 4)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$3/4,3/4,0$
[2] $P4_1$ (76)	1; 2; 3; 4		$3/4,1/4,0$

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$I4_1$ (80)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2})\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$I4_1$ (80)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4})\rangle$ $p>4$; $p\equiv 1 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$I4_1$ (80)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4})\rangle$ $p>2$; $p\equiv 3 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,0$
$[p^2]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$I4_1$ (80)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)$; $3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$I4_1$ (80)	$\langle 2+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+2u,-\frac{r}{2}+\frac{q}{2}-\frac{1}{2},0)$; $3+(\frac{r}{2}+u,\frac{q}{2}-u-\frac{1}{2},0)\rangle$ $q>0$; $r>1$; q odd; r even; $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$
$I4_1$ (80)	$\langle 2+(\frac{q}{2}+\frac{r}{2}+\frac{1}{2}+2u,-\frac{r}{2}+\frac{q}{2}-\frac{1}{2},0)$; $3+(\frac{r}{2}+\frac{1}{2}+u,\frac{q}{2}-1-u,0)\rangle$ $q>1$; $r>0$; q even; r odd; $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$1/2+u,0,0$

I Minimal *translationengleiche* supergroups

[2] $I4_1/a$ (88); [2] $I4_122$ (98); [2] $I4_1md$ (109); [2] $I4_1cd$ (110)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2$ (77, $P4_2$)

$P\bar{4}$ No. 81 $P\bar{4}$ S_4^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
4	h	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $y,\bar{x},\bar{z}$ (4) $\bar{y},x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P2$ (3, $P112$) 1; 2

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P\bar{4}$ (81)	$\langle 2;\ 3 \rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,1) \rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$C\bar{4}$ (81, $P\bar{4}$)	$\langle 2;\ 3 \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}$ (81, $P\bar{4}$)	$\langle 2+(1,1,0);\ 3+(0,1,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$F\bar{4}$ (82, $I\bar{4}$)	$\langle 2;\ 3 \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F\bar{4}$ (82, $I\bar{4}$)	$\langle 2;\ 3+(0,0,1) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P\bar{4}$ (81)	$\langle 2;\ 3 \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,2) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,4) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$P\bar{4}$ (81)	$\langle 2;\ 3+(0,0,2u) \rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P\bar{4}$ (81)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0) \rangle$ $p>2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p = q^2+r^2]$ $\mathbf{a}' = q\mathbf{a}-r\mathbf{b},\ \mathbf{b}' = r\mathbf{a}+q\mathbf{b}$			
$P\bar{4}$ (81)	$\langle 2+(2u,0,0);\ 3+(u,u,0) \rangle$ $q>0;\ r>0;\ p>4;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4/m$ (83); [2] $P4_2/m$ (84); [2] $P4/n$ (85); [2] $P4_2/n$ (86); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2c$ (112); [2] $P\bar{4}2_1m$ (113); [2] $P\bar{4}2_1c$ (114); [2] $P\bar{4}m2$ (115); [2] $P\bar{4}c2$ (116); [2] $P\bar{4}b2$ (117); [2] $P\bar{4}n2$ (118)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I\bar{4}$ (82)

- **Decreased unit cell** none

S_4^2 $I\bar{4}$ No. 82 $I\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
8	g	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $y,\bar{x},\bar{z}$ (4) $\bar{y},x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $I2$ (5, $A112$)	$(1;\ 2)+$	$\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P\bar{4}$ (81)	1; 2; 3; 4		
[2] $P\bar{4}$ (81)	1; 2; $(3;\ 4)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/2, 0, 1/4

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I\bar{4}$ (82)	$\langle 2;\ 3\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$I\bar{4}$ (82)	$\langle 2;\ 3+(0,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$I\bar{4}$ (82)	$\langle 2;\ 3+(0,0,4)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$

$I\bar{4}$ (82)	$\langle 2;\ 3+(0,0,2u)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$

$I\bar{4}$ (82)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0)\rangle$ $p>2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3 \pmod 4$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u,v,0$

$[p = q^2 + r^2]$ $\mathbf{a}' = q\mathbf{a} - r\mathbf{b},\ \mathbf{b}' = r\mathbf{a} + q\mathbf{b}$

$I\bar{4}$ (82)	$\langle 2+(2u,0,0);\ 3+(u,u,0)\rangle$ $q>0;\ r>0;\ p>4;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b}, r\mathbf{a}+q\mathbf{b}, \mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $I4/m$ (87); [2] $I4_1/a$ (88); [2] $I\bar{4}m2$ (119); [2] $I\bar{4}c2$ (120); [2] $I\bar{4}2m$ (121); [2] $I\bar{4}2d$ (122)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C\bar{4}$ (81, $P\bar{4}$)

$P4/m$ No. 83 $P4/m$ C_{4h}^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y},x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8
[2] $P4$ (75)	1; 2; 3; 4
[2] $P2/m$ (10, $P112/m$)	1; 2; 5; 6

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2/m$ (84)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/m$ (84)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/m$ (83)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/m$ (83)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$C4/e$ (85, $P4/n$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4/e$ (85, $P4/n$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4/m$ (83, $P4/m$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4/m$ (83, $P4/m$)	$\langle (2;\ 5)+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b},\ \mathbf{c}' = 2\mathbf{c}$			
$F4/m$ (87, $I4/m$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4/m$ (87, $I4/m$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F4/m$ (87, $I4/m$)	$\langle (2;\ 5)+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4/m$ (87, $I4/m$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(1,1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4/m$ (83)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/m$ (83)	$\langle 2;\ 3;\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/m$ (83)	$\langle 2;\ 3;\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P4/m$ (83)	$\langle 2;\ 3;\ 5+(0,0,2u)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P4/m$ (83)	$\langle (2;\ 5)+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p>2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p = q^2+r^2$] $\mathbf{a}' = q\mathbf{a}-r\mathbf{b},\ \mathbf{b}' = r\mathbf{a}+q\mathbf{b}$			
$P4/m$ (83)	$\langle (2;\ 5)+(2u,0,0);\ 3+(u,-u,0)\rangle$ $q>0;\ r>0;\ p>4;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 1$ (mod 4)	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4/mcc$ (124); [2] $P4/mbm$ (127); [2] $P4/mnc$ (128)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4/m$ (87)

- **Decreased unit cell** none

C_{4h}^2 $P4_2/m$ No. 84 $P4_2/m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $y,\bar{x},\bar{z}+\frac{1}{2}$	(8) $\bar{y},x,\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		0,0,1/4
[2] $P4_2$ (77)	1; 2; 3; 4		
[2] $P2/m$ (10, $P112/m$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$

$C4_2/e$ (86, $P4_2/n$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	0,1/2,0
$C4_2/e$ (86, $P4_2/n$)	$\langle 2+(1,1,0);\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	1/2,0,0
$C4_2/m$ (84, $P4_2/m$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2/m$ (84, $P4_2/m$)	$\langle (2;\ 5)+(1,1,0);\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	1/2,1/2,0

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/m$ (84)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/m$ (84)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,1
$P4_2/m$ (84)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/m$ (84)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/m$ (84)	$\langle (2;\ 5)+(2u,2v,0);\ 3+(u+v,-u+v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3\ (\mathrm{mod}\ 4)$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

[$p=q^2+r^2$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+q\mathbf{b}$

$P4_2/m$ (84)	$\langle (2;\ 5)+(u,u,0);\ 3+(u,0,0)\rangle$ $q>0;\ r>0;\ p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1\ (\mathrm{mod}\ 4)$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/mmc$ (131); [2] $P4_2/mcm$ (132); [2] $P4_2/mbc$ (135); [2] $P4_2/mnm$ (136)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4/m$ (87)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/m$ (83)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 85, pp. 208–209.

$P4/n$ No. 85 $P4/n$ C_{4h}^3

ORIGIN CHOICE 1, Origin at $\bar{4}$ on n, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y},x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		
[2] $P4$ (75)	1; 2; 3; 4		$1/2,0,0$
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/n$ (86)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_2/n$ (86)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/n$ (85)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P4/n$ (85)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/n$ (85)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$P4/n$ (85)	$\langle 2+(2u,0,0);\ 3+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2}-u,0);$ $5+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0)\rangle$ $q>0;\ r>0;\ p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/m$ (83, $P4/m$); [2] $I4/m$ (87)

- **Decreased unit cell** none

C_{4h}^{3} $P4/n$ No. 85 $P4/n$

ORIGIN CHOICE 2, Origin at $\bar{1}$ on n, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
8	g	1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (3) $\bar{y}+\frac{1}{2},x,z$ (4) $y,\bar{x}+\frac{1}{2},z$ (5) $\bar{x},\bar{y},\bar{z}$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $y+\frac{1}{2},\bar{x},\bar{z}$ (8) $\bar{y},x+\frac{1}{2},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		$1/4,3/4,0$
[2] $P4$ (75)	1; 2; 3; 4		$1/4,1/4,0$
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/2,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/n$ (86)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$P4_2/n$ (86)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$P4/n$ (85)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P4/n$ (85)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4/n$ (85)	$\langle 2;\ 3;\ 5+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/n$ (85)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(2u,2v,0)\rangle$ $p>2;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for prime $p\equiv 3\ (\mathrm{mod}\ 4)$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$P4/n$ (85)	$\langle 2+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0);$ $3+(\frac{q}{2}-\frac{1}{2}+u,-\frac{r}{2}-u,0);\ 5+(2u,0,0)\rangle$ $q>0;\ q$ odd; $r>1;\ r$ even; $p>4;\ 0\leq u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$
$P4/n$ (85)	$\langle 2+(\frac{q}{2}+\frac{r}{2}+\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0);$ $3+(\frac{q}{2}+u,-\frac{r}{2}-\frac{1}{2}-u,0);\ 5+(1+2u,0,0)\rangle$ $q>1;\ q$ even; $r>0;\ r$ odd; $p>4;\ 0\leq u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$1/2+u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/m$ (83, $P4/m$); [2] $I4/m$ (87)

- **Decreased unit cell** none

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 86, pp. 210–211.

$P4_2/n$ No. 86 $P4_2/n$ C_{4h}^4

ORIGIN CHOICE 1, Origin at $\bar{4}$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y},x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		
[2] $P4_2$ (77)	1; 2; 3; 4		$1/2,0,0$
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/4,1/4,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P4_2/n$ (86)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P4_2/n$ (86)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P4_2/n$ (86)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_2/n$ (86)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P4_2/n$ (86)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3\ (\mathrm{mod}\ 4)$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$P4_2/n$ (86)	$\langle 2+(2u,0,0);\ 3+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2}-u,0);$ $5+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0)\rangle$ $q>0;\ r>0;\ p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1\ (\mathrm{mod}\ 4)$	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/m$ (84, $P4_2/m$); [2] $I4/m$ (87)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/n$ (85)

ORIGIN CHOICE 2, Origin at $\bar{1}$ on n, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
8 g 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$
	(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}$ (81)	1; 2; 7; 8		1/4, 1/4, 1/4
[2] $P4_2$ (77)	1; 2; 3; 4		3/4, 1/4, 0
[2] $P2/n$ (13, $P112/a$)	1; 2; 5; 6	$-\mathbf{a}-\mathbf{b},\mathbf{a},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	0, 0, 1/2
$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	1/2, 1/2, 0
$F4_1/d$ (88, $I4_1/a$)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	1/2, 1/2, 1/2

[3] $\mathbf{c}'=3\mathbf{c}$

{ $P4_2/n$ (86)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P4_2/n$ (86)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
{ $P4_2/n$ (86)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/n$ (86)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/n$ (86)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)$; $3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);\ 5+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

[$p=q^2+r^2$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+q\mathbf{b}$

$P4_2/n$ (86)	$\langle 2+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0)$; $3+(\frac{r}{2}+u,\frac{q}{2}-\frac{1}{2}-u,0);\ 5+(2u,0,0)\rangle$ $q>0;\ q$ odd; $r>1;\ r$ even; $p>4;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$
$P4_2/n$ (86)	$\langle 2+(\frac{q}{2}+\frac{r}{2}+\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0)$; $3+(\frac{r}{2}+\frac{1}{2}+u,\frac{q}{2}-1-u,0);\ 5+(1+2u,0,0)\rangle$ $q>1;\ q$ even; $r>0;\ r$ odd; $p>4;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$1/2+u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/m$ (84, $P4_2/m$); [2] $I4/m$ (87)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/n$ (85)

$I4/m$ No. 87 $I4/m$ C_{4h}^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
16	i	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$
			(5) $\bar{x},\bar{y},\bar{z}$ (6) $x,y,\bar{z}$ (7) $y,\bar{x},\bar{z}$ (8) $\bar{y},x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+		
[2] $I4$ (79)	(1; 2; 3; 4)+		
[2] $I2/m$ (12, $A112/m$)	(1; 2; 5; 6)+	$\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$	

II Maximal *klassengleiche* subgroups

• **Loss of centring translations**

[2] $P4_2/n$ (86)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $P4/n$ (85)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $P4_2/m$ (84)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4/m$ (83)	1; 2; 3; 4; 5; 6; 7; 8		

• **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4/m$ (87)	$\langle 2;\ 3;\ 5 \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I4/m$ (87)	$\langle 2;\ 3;\ 5+(0,0,2) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I4/m$ (87)	$\langle 2;\ 3;\ 5+(0,0,4) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I4/m$ (87)	$\langle 2;\ 3;\ 5+(0,0,2u) \rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$I4/m$ (87)	$\langle (2;\ 5)+(2u,2v,0);\ 3+(u+v,-u+v,0) \rangle$ $p>2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

[$p = q^2+r^2$] $\mathbf{a}' = q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}' = r\mathbf{a}+q\mathbf{b}$

$I4/m$ (87)	$\langle (2;\ 5)+(2u,0,0);\ 3+(u,-u,0) \rangle$ $q>0;\ r>0;\ p>4;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 1$ (mod 4)	$q\mathbf{a}-r\mathbf{b}, r\mathbf{a}+q\mathbf{b}, \mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $I4/mmm$ (139); [2] $I4/mcm$ (140)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations** none

• **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4/m$ (83, $P4/m$)

C_{4h}^6 $I4_1/a$ No. 88 $I4_1/a$

ORIGIN CHOICE 1, Origin at $\bar{4}$, at $0,-\frac{1}{4},-\frac{1}{8}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16 f 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
	(5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+		
[2] $I4_1$ (80)	(1; 2; 3; 4)+		
[2] $I2/a$ (15, $A112/a$)	(1; 2; 5; 6)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,1/4,1/8$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_1/a$ (88)	$\langle(2;\ 5)+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2})\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1/4$
$I4_1/a$ (88)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,5/4$
$I4_1/a$ (88)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,9/4$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$I4_1/a$ (88)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});\ 5+(0,0,\frac{p}{4}-\frac{1}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$I4_1/a$ (88)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});$ $5+(1,0,\frac{p}{4}+\frac{1}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,1/4+u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$I4_1/a$ (88)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);\ 5+(2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

$[p=q^2+r^2]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+q\mathbf{b}$

$I4_1/a$ (88)	$\langle 2+(\frac{q}{2}+\frac{r}{2}-\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0);$ $3+(\frac{r}{2}+u,\frac{q}{2}-\frac{1}{2}-u,0);\ 5+(\frac{r}{2}+2u,\frac{q}{2}-\frac{1}{2},0)\rangle$ $q>0;\ r>1;\ p>4;\ 0\le u<p$ p conjugate subgroups for odd q and prime $p\equiv 1$ (mod 4)	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$
$I4_1/a$ (88)	$\langle 2+(\frac{q}{2}+\frac{r}{2}+\frac{1}{2}+2u,\frac{q}{2}-\frac{r}{2}-\frac{1}{2},0);$ $3+(\frac{r}{2}+\frac{1}{2}+u,\frac{q}{2}-1-u,0);\ 5+(\frac{r}{2}+1+2u,\frac{q}{2}-\frac{1}{2},\frac{1}{2})\rangle$ $q>1;\ r>0;\ p>4;\ 0\le u<p$ p conjugate subgroups for even q and prime $p\equiv 1$ (mod 4)	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$1/2+u,0,1/4$

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2/e$ (86, $P4_2/n$)

ORIGIN CHOICE 2, Origin at $\bar{1}$ on glide plane b, at $0,\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
16 f 1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (3) $\bar{y}+\frac{3}{4},x+\frac{1}{4},z+\frac{1}{4}$ (4) $y+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$
	(5) $\bar{x},\bar{y},\bar{z}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $y+\frac{1}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$ (8) $\bar{y}+\frac{1}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}$ (82)	(1; 2; 7; 8)+		0, 1/4, 5/8
[2] $I4_1$ (80)	(1; 2; 3; 4)+		1/2, 1/4, 0
[2] $I2/a$ (15, $A112/a$)	(1; 2; 5; 6)+	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_1/a$ (88)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,0)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	1/2, 0, 0
$I4_1/a$ (88)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	1/2, 0, 1
$I4_1/a$ (88)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	1/2, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1/a$ (88)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});\ 5+(0,0,2u)\rangle$ $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$I4_1/a$ (88)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});\ 5+(1,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$I4_1/a$ (88)	$\langle 2+(\frac{p}{2}+\frac{1}{2}+2u,2v,0);$ $3+(\frac{3p}{4}-\frac{1}{4}+u+v,\frac{p}{4}-\frac{3}{4}-u+v,0);\ 5+(1+2u,2v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$1/2+u,v,0$

[$p=q^2+r^2$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+q\mathbf{b}$

$I4_1/a$ (88)	$\langle 2+(\frac{q}{2}+\frac{1}{2}+2u,-\frac{r}{2},0);$ $3+(\frac{3q}{4}+\frac{r}{4}-\frac{1}{4}+u,\frac{q}{4}-\frac{3r}{4}-\frac{3}{4}-u,0);\ 5+(1+2u,0,0)\rangle$ $q>0$; $r>1$; $p>4$; $0\le u<p$; q odd; $q+r=3$ (mod 4) p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$1/2+u,0,0$
$I4_1/a$ (88)	$\langle 2+(\frac{q}{2}-\frac{1}{2}+2u,-\frac{r}{2},0);$ $3+(\frac{3q}{4}+\frac{r}{4}-\frac{3}{4}+u,\frac{q}{4}-\frac{3r}{4}-\frac{1}{4}-u,0);\ 5+(2u,0,0)\rangle$ $q>0$; $r>1$; $p>12$; $0\le u<p$; q odd; $q+r=1$ (mod 4) p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$
$I4_1/a$ (88)	$\langle 2+(\frac{q}{2}+1+2u,-\frac{r}{2}+\frac{1}{2},0);$ $3+(\frac{3q}{4}+\frac{r}{4}+\frac{1}{4}+u,\frac{q}{4}-\frac{3r}{4}-\frac{3}{4}-u,0);\ 5+(\frac{3}{2}+2u,\frac{1}{2},\frac{1}{2})\rangle$ $q>1$; $r>0$; $p>4$; $0\le u<p$; q even; $q+r=3$ (mod 4) p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$3/4+u,1/4,1/4$
$I4_1/a$ (88)	$\langle 2+(\frac{q}{2}+2u,-\frac{r}{2}+\frac{1}{2},0);$ $3+(\frac{3q}{4}+\frac{r}{4}-\frac{1}{4}+u,\frac{q}{4}-\frac{3r}{4}-\frac{1}{4}-u,0);\ 5+(\frac{1}{2}+2u,\frac{1}{2},\frac{1}{2})\rangle$ $q>1$; $r>0$; $p>12$; $0\le u<p$; q even; $q+r=1$ (mod 4) p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$1/4+u,1/4,1/4$

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2/e$ (86, $P4_2/n$)

D_4^1 $P422$ No. 89 $P422$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P411$ (75, $P4$)	1; 2; 3; 4		
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P221$ (16, $P222$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_222$ (93)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_222$ (93)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P422$ (89)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P422$ (89)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C422_1$ (90, $P42_12$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C422_1$ (90, $P42_12$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C422$ (89, $P422$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C422$ (89, $P422$)	$\langle 2+(1,1,0);\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F422$ (97, $I422$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F422$ (97, $I422$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F422$ (97, $I422$)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F422$ (97, $I422$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P422$ (89)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P422$ (89)	$\langle 2;\ 3;\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P422$ (89)	$\langle 2;\ 3;\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P422$ (89)	$\langle 2;\ 3;\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P422$ (89)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4/mcc$ (124); [2] $P4/nbm$ (125); [2] $P4/nnc$ (126); [3] $P432$ (207)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I422$ (97)

- **Decreased unit cell** none

$P42_12$ No. 90 $P42_12$ D_4^2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
8 g 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$
	(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P411$ (75, $P4$)	1; 2; 3; 4		$0,1/2,0$
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P22_11$ (18, $P2_12_12$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_22_12$ (94)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_22_12$ (94)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P42_12$ (90)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P42_12$ (90)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P42_12$ (90)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P42_12$ (90)	$\langle 2;\ 3;\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P42_12$ (90)	$\langle 2;\ 3;\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P42_12$ (90)	$\langle 2;\ 3;\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P42_12$ (90)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mbm$ (127); [2] $P4/mnc$ (128); [2] $P4/nmm$ (129); [2] $P4/ncc$ (130)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C422$ (89, $P422$); [2] $I422$ (97)

- **Decreased unit cell** none

D_4^3 $P4_122$ No. 91 $P4_122$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{3}{4}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $P4_111$ (76, $P4_1$)	1; 2; 3; 4		
[2] $P2_121$ (17, $P222_1$)	1; 2; 5; 6		0, 0, 1/4
[2] $P2_112$ (20, $C222_1$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	0, 0, 1/8

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
$C4_122_1$ (92, $P4_12_12$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	1/2, 1/2, 1/4
$C4_122_1$ (92, $P4_12_12$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	0, 0, 1/4
$C4_122$ (91, $P4_122$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	0, 0, 3/8
$C4_122$ (91, $P4_122$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(1,0,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	1/2, 1/2, 3/8
[3] $\mathbf{c}'=3\mathbf{c}$			
$\{$ $P4_322$ (95)	$\langle 5;\ 2+(0,0,1);\ 3+(0,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P4_322$ (95)	$\langle 2+(0,0,1);\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P4_322$ (95)	$\langle 2+(0,0,1);\ 3+(0,0,2);\ 5+(0,0,4)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_322$ (95)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{3p}{4}-\frac{1}{4});\ 5+(0,0,2u)\rangle$ $p>2$; $0\leq u<p$ p conjugate subgroups for prime $p\equiv 3 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$
$P4_122$ (91)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});\ 5+(0,0,2u)\rangle$ $p>4$; $0\leq u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P4_122$ (91)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0)\rangle$ $p>2$; $0\leq u<p$; $0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4_122$ (98)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4_222$ (93)

$P4_12_12$ No. 92 $P4_12_12$ D_4^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{3}{4}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{4}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{3}{4}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P4_111$ (76, $P4_1$)	1; 2; 3; 4		$0,1/2,0$
[2] $P2_112$ (20, $C222_1$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/4$
[2] $P2_12_11$ (19, $P2_12_12_1$)	1; 2; 5; 6		$1/4,0,3/8$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_32_12$ (96)	$\langle 2+(0,0,1);\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_32_12$ (96)	$\langle 2+(0,0,1);\ 3+(0,0,2);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_32_12$ (96)	$\langle 2+(0,0,1);\ 3+(0,0,2);\ 5+(0,0,6)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_32_12$ (96)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{3p}{4}-\frac{1}{4});$ $5+(0,0,\frac{3p}{4}-\frac{1}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3\ (\mathrm{mod}\ 4)$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P4_12_12$ (92)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});$ $5+(0,0,\frac{p}{4}-\frac{1}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1\ (\mathrm{mod}\ 4)$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$P4_12_12$ (92)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $P4_132$ (213)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_122$ (91, $P4_122$); [2] $I4_122$ (98)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4_22_12$ (94)

D_4^5 $P4_222$ No. 93 $P4_222$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P4_211$ (77, $P4_2$)	1; 2; 3; 4		
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/4$
[2] $P221$ (16, $P222$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_322$ (95)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_322$ (95)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_122$ (91)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_122$ (91)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4_222_1$ (94, $P4_22_12$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_222_1$ (94, $P4_22_12$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4_222$ (93, $P4_222$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/4$
$C4_222$ (93, $P4_222$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(1,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,1/4$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F4_122$ (98, $I4_122$)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$F4_122$ (98, $I4_122$)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$F4_122$ (98, $I4_122$)	$\langle (2;\ 3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,0,0$
$F4_122$ (98, $I4_122$)	$\langle (2;\ 3)+(1,0,0);\ 5+(1,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_222$ (93)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_222$ (93)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_222$ (93)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_222$ (93)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_222$ (93)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/mmc$ (131); [2] $P4_2/mcm$ (132); [2] $P4_2/nbc$ (133); [2] $P4_2/nnm$ (134); [3] $P4_232$ (208)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I422$ (97)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P422$ (89)

$P4_22_12$ No. 94 $P4_22_12$ D_4^6

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P4_211$ (77, $P4_2$)	1; 2; 3; 4		$0,1/2,0$
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a-b},\mathbf{a+b},\mathbf{c}$	
[2] $P22_11$ (18, $P2_12_12$)	1; 2; 5; 6		$0,0,1/4$

II Maximal *klassengleiche* subgroups

• **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$

$P4_32_12$ (96)	$\langle 5;\ (2;\ 3)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_32_12$ (96)	$\langle (2;\ 3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_12_12$ (92)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_12_12$ (92)	$\langle 3;\ (2;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_22_12$ (94)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_22_12$ (94)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_22_12$ (94)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_22_12$ (94)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_22_12$ (94)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/mbc$ (135); [2] $P4_2/mnm$ (136); [2] $P4_2/nmc$ (137); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations**

[2] $C4_222$ (93, $P4_222$); [2] $I422$ (97)

• **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P42_12$ (90)

D_4^7 $P4_322$ No. 95 $P4_322$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{3}{4}$	(4) $y,\bar{x},z+\frac{1}{4}$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{4}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $P4_311$ (78, $P4_3$)	1; 2; 3; 4		
[2] $P2_112$ (20, $C222_1$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,3/8$
[2] $P2_121$ (17, $P222_1$)	1; 2; 5; 6		$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4_322_1$ (96, $P4_32_12$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/4$
$C4_322_1$ (96, $P4_32_12$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,1/4$
$C4_322$ (95, $P4_322$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/8$
$C4_322$ (95, $P4_322$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(1,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,1/8$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_122$ (91)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_122$ (91)	$\langle 3;\ 2+(0,0,1);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_122$ (91)	$\langle 3;\ 2+(0,0,1);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_322$ (95)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{3p}{4}-\frac{3}{4});\ 5+(0,0,2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P4_122$ (91)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{3}{4});\ 5+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3 \pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_322$ (95)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4_122$ (98)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4_222$ (93)

$P4_32_12$ No. 96 $P4_32_12$ D_4^8

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

8	*b*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{3}{4}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{4}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P4_311$ (78, $P4_3$)	1; 2; 3; 4		0,1/2,0
[2] $P2_112$ (20, $C222_1$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	0,0,1/4
[2] $P2_12_11$ (19, $P2_12_12_1$)	1; 2; 5; 6		1/4,0,1/8

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_12_12$ (92)	$\langle 3;\ 5;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_12_12$ (92)	$\langle 3;\ 2+(0,0,1);\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,1
$P4_12_12$ (92)	$\langle 3;\ 2+(0,0,1);\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$P4_32_12$ (96)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{3p}{4}-\frac{3}{4});$ $5+(0,0,\frac{3p}{4}-\frac{3}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P4_12_12$ (92)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{3}{4});$ $5+(0,0,\frac{p}{4}-\frac{3}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_32_12$ (96)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $P4_332$ (212)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_322$ (95, $P4_322$); [2] $I4_122$ (98)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4_22_12$ (94)

D_4^9 $I422$ No. 97 $I422$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $I411$ (79, $I4$)	$(1;\ 2;\ 3;\ 4)+$		
[2] $I221$ (23, $I222$)	$(1;\ 2;\ 5;\ 6)+$		
[2] $I212$ (22, $F222$)	$(1;\ 2;\ 7;\ 8)+$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_22_12$ (94)	$1;\ 2;\ 7;\ 8;\ (3;\ 4;\ 5;\ 6)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4_222$ (93)	$1;\ 2;\ 5;\ 6;\ (3;\ 4;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P42_12$ (90)	$1;\ 2;\ 3;\ 4;\ (5;\ 6;\ 7;\ 8)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,1/4$
[2] $P422$ (89)	$1;\ 2;\ 3;\ 4;\ 5;\ 6;\ 7;\ 8$		

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I422$ (97)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I422$ (97)	$\langle 2;\ 3;\ 5+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I422$ (97)	$\langle 2;\ 3;\ 5+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I422$ (97)	$\langle 2;\ 3;\ 5+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$I422$ (97)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $F432$ (209); [3] $I432$ (211)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C422$ (89, $P422$)

$I4_122$ No. 98 $I4_122$ D_4^{10}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $I4_111$ (80, $I4_1$)	(1; 2; 3; 4)+		
[2] $I2_121$ (24, $I2_12_12_1$)	(1; 2; 5; 6)+		$0,1/4,3/8$
[2] $I2_112$ (22, $F222$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

• **Loss of centring translations**

[2] $P4_32_12$ (96)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,3/4,1/4$
[2] $P4_322$ (95)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,3/8$
[2] $P4_12_12$ (92)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,0$
[2] $P4_122$ (91)	1; 2; 3; 4; 5; 6; 7; 8		$3/4,1/4,3/8$

• **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_122$ (98)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1/4$
$I4_122$ (98)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,5/4$
$I4_122$ (98)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,6)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,9/4$

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_122$ (98)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},\frac{1}{2}-1,\frac{1}{2}+\frac{p}{4}-\frac{3}{4});$ $5+(1,0,\frac{3p}{4}-\frac{1}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3 \pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,1/4+u$
$I4_122$ (98)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});$ $5+(0,0,\frac{3p}{4}-\frac{3}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$I4_122$ (98)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $F4_132$ (210); [3] $I4_132$ (214)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations** none

• **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_222$ (93, $P4_222$)

C_{4v}^{1} $P4mm$ No. 99 $P4mm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P411$ (75, $P4$)	1; 2; 3; 4		
[2] $P21m$ (35, $Cmm2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2m1$ (25, $Pmm2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2mc$ (105)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4cc$ (103)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2cm$ (101)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4md$ (100, $P4bm$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4md$ (100, $P4bm$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4mm$ (99, $P4mm$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4mm$ (99, $P4mm$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F4mc$ (108, $I4cm$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4mc$ (108, $I4cm$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4mm$ (107, $I4mm$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4mm$ (107, $I4mm$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P4mm$ (99)	$\langle 2;\ 3;\ 5\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4mm$ (99)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4/nmm$ (129)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4mm$ (107)

- **Decreased unit cell** none

$P4bm$ No. 100 $P4bm$ C_{4v}^2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P411$ (75, $P4$)	1; 2; 3; 4		
[2] $P21m$ (35, $Cmm2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2b1$ (32, $Pba2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2bc$ (106)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4nc$ (104)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2nm$ (102)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$P4bm$ (100)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4bm$ (100)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4bm$ (100)	$\langle 2;\ 3;\ 5\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4bm$ (100)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4/mbm$ (127)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4mm$ (99, $P4mm$); [2] $I4cm$ (108)

- **Decreased unit cell** none

C_{4v}^{3} $P4_2cm$ No. 101 $P4_2cm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*e*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P4_211$ (77, $P4_2$)	1; 2; 3; 4		
[2] $P21m$ (35, $Cmm2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2c1$ (27, $Pcc2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4_2cd$ (106, $P4_2bc$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2cd$ (106, $P4_2bc$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	1/2, 1/2, 0
$C4_2cm$ (105, $P4_2mc$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2cm$ (105, $P4_2mc$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	1/2, 1/2, 0
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_2cm$ (101)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_2cm$ (101)	$\langle 2;\ (3;\ 5)+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_2cm$ (101)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/mcm$ (132); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2cm$ (105, $P4_2mc$); [2] $I4cm$ (108)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4mm$ (99)

$P4_2nm$ No. 102 $P4_2nm$ C_{4v}^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P4_211$ (77, $P4_2$)	1; 2; 3; 4		$0,1/2,0$
[2] $P21m$ (35, $Cmm2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2n1$ (34, $Pnn2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F4_1dc$ (110, $I4_1cd$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4_1dc$ (110, $I4_1cd$)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4_1dm$ (109, $I4_1md$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4_1dm$ (109, $I4_1md$)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_2nm$ (102)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_2nm$ (102)	$\langle 2;\ (3;\ 5)+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_2nm$ (102)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/nnm$ (134); [2] $P4_2/mnm$ (136)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2cm$ (105, $P4_2mc$); [2] $I4mm$ (107)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4bm$ (100)

C_{4v}^{5} $P4cc$ No. 103 $P4cc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P411$ (75, $P4$)	1; 2; 3; 4		
[2] $P21c$ (37, $Ccc2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2c1$ (27, $Pcc2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4cd$ (104, $P4nc$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4cd$ (104, $P4nc$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4cc$ (103, $P4cc$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4cc$ (103, $P4cc$)	$\langle 2+(1,1,0);\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4cc$ (103)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4cc$ (103)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4cc$ (103)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mcc$ (124); [2] $P4/ncc$ (130)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4cm$ (108)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4mm$ (99)

$P4nc$ No. 104 $P4nc$ C_{4v}^{6}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P411$ (75, $P4$)	1; 2; 3; 4		
[2] $P21c$ (37, $Ccc2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2n1$ (34, $Pnn2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4nc$ (104)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4nc$ (104)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$P4nc$ (104)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/nnc$ (126); [2] $P4/mnc$ (128)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4cc$ (103, $P4cc$); [2] $I4mm$ (107)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4bm$ (100)

C_{4v}^{7} $P4_2mc$ No. 105 $P4_2mc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P4_211$ (77, $P4_2$)	1; 2; 3; 4		
[2] $P21c$ (37, $Ccc2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2m1$ (25, $Pmm2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4_2md$ (102, $P4_2nm$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4_2md$ (102, $P4_2nm$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2mc$ (101, $P4_2cm$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2mc$ (101, $P4_2cm$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_2mc$ (105)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_2mc$ (105)	$\langle 2;\ 5;\ 3+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_2mc$ (105)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/mmc$ (131); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2mc$ (101, $P4_2cm$); [2] $I4mm$ (107)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4mm$ (99)

$P4_2bc$ No. 106 $P4_2bc$ C_{4v}^8

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P4_211$ (77, $P4_2$)	1; 2; 3; 4		
[2] $P21c$ (37, $Ccc2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2b1$ (32, $Pba2$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2bc$ (106)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2bc$ (106)	$\langle 2;\ 5;\ 3+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2bc$ (106)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4_2/nbc$ (133); [2] $P4_2/mbc$ (135)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2mc$ (101, $P4_2cm$); [2] $I4cm$ (108)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4bm$ (100)

C_{4v}^{9} $I4mm$ No. 107 $I4mm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
16	e	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y},x,z$ (4) $y,\bar{x},z$
			(5) $x,\bar{y},z$ (6) $\bar{x},y,z$ (7) $\bar{y},\bar{x},z$ (8) y,x,z

I Maximal *translationengleiche* subgroups

[2] $I411$ (79, $I4$)	(1; 2; 3; 4)+		
[2] $I2m1$ (44, $Imm2$)	(1; 2; 5; 6)+		
[2] $I21m$ (42, $Fmm2$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2mc$ (105)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4nc$ (104)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4_2nm$ (102)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4mm$ (99)	1; 2; 3; 4; 5; 6; 7; 8		

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4mm$ (107)	$\langle 2; 3; 5 \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I4mm$ (107)	$\langle 2; 3; 5 \rangle$ $p > 2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

[p^2] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$I4mm$ (107)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0) \rangle$ $p > 2$; $0 \le u < p$; $0 \le v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4/mmm$ (139)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4mm$ (99, $P4mm$)

$I4cm$ No. 108 $I4cm$ C_{4v}^{10}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $I411$ (79, $I4$)	(1; 2; 3; 4)+		
[2] $I2c1$ (45, $Iba2$)	(1; 2; 5; 6)+		
[2] $I21m$ (42, $Fmm2$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2bc$ (106)	1; 2; 7; 8; (3; 4; 5; 6) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4cc$ (103)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4_2cm$ (101)	1; 2; 5; 6; (3; 4; 7; 8) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4bm$ (100)	1; 2; 3; 4; (5; 6; 7; 8) $+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4cm$ (108)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4cm$ (108)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$I4cm$ (108)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(0,2v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4/mcm$ (140)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4mm$ (99, $P4mm$)

C_{4v}^{11} $I4_1md$ No. 109 $I4_1md$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16 c 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
	(5) $x,\bar{y},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	(8) $y+\frac{1}{2},x,z+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $I4_111$ (80, $I4_1$)	(1; 2; 3; 4)+		
[2] $I2m1$ (44, $Imm2$)	(1; 2; 5; 6)+		
[2] $I21d$ (43, $Fdd2$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_1md$ (109)	$\langle 5;\ 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2})\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1md$ (109)	$\langle 5;\ 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4})\rangle$ $p>2$; $p\equiv 3 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,0$

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1md$ (109)	$\langle 5;\ 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4})\rangle$ $p>4$; $p\equiv 1 \pmod 4$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$I4_1md$ (109)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)$; $3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0)$; $5+(0,2v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2md$ (102, $P4_2nm$)

$I4_1cd$ No. 110 $I4_1cd$ C_{4v}^{12}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	*b*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(8) $y+\frac{1}{2},x,z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $I4_111$ (80, $I4_1$)	(1; 2; 3; 4)+	
[2] $I2c1$ (45, $Iba2$)	(1; 2; 5; 6)+	
[2] $I21d$ (43, $Fdd2$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_1cd$ (110)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	1/2, 0, 0

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1cd$ (110)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});$ $5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2;\ p\equiv 3\ (\mathrm{mod}\ 4)$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	1/2, 0, 0

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1cd$ (110)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});$ $5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>4;\ p\equiv 1\ (\mathrm{mod}\ 4)$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$I4_1cd$ (110)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4_1/acd$ (142)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2md$ (102, $P4_2nm$)

D^1_{2d} $P\bar{4}2m$ No. 111 $P\bar{4}2m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	o	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P21m$ (35, $Cmm2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P221$ (16, $P222$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

• **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{4}2c$ (112)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}2c$ (112)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{4}2m$ (111)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}2m$ (111)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C\bar{4}2d$ (117, $P\bar{4}b2$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}2d$ (117, $P\bar{4}b2$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C\bar{4}2m$ (115, $P\bar{4}m2$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}2m$ (115, $P\bar{4}m2$)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F\bar{4}2c$ (120, $I\bar{4}c2$)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F\bar{4}2c$ (120, $I\bar{4}c2$)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F\bar{4}2m$ (119, $I\bar{4}m2$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F\bar{4}2m$ (119, $I\bar{4}m2$)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{4}2m$ (111)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{4}2m$ (111)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{4}2m$ (111)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

• **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P\bar{4}2m$ (111)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{4}2m$ (111)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4/nbm$ (125); [2] $P4_2/mcm$ (132); [2] $P4_2/nnm$ (134); [3] $P\bar{4}3m$ (215)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations**

[2] $C\bar{4}2m$ (115, $P\bar{4}m2$); [2] $I\bar{4}2m$ (121)

• **Decreased unit cell** none

$P\bar{4}2c$ No. 112 $P\bar{4}2c$ D_{2d}^{2}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

8	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P21c$ (37, $Ccc2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P221$ (16, $P222$)	1; 2; 5; 6		$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C\bar{4}2d$ (118, $P\bar{4}n2$)	$\langle 2;\ 3;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}2d$ (118, $P\bar{4}n2$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C\bar{4}2c$ (116, $P\bar{4}c2$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}2c$ (116, $P\bar{4}c2$)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P\bar{4}2c$ (112)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{4}2c$ (112)	$\langle 2;\ 3+(0,0,2);\ 5+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{4}2c$ (112)	$\langle 2;\ 3+(0,0,4);\ 5+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P\bar{4}2c$ (112)	$\langle 2;\ 3+(0,0,2u);\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{4}2c$ (112)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mcc$ (124); [2] $P4/nnc$ (126); [2] $P4_2/mmc$ (131); [2] $P4_2/nbc$ (133); [3] $P\bar{4}3n$ (218)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C\bar{4}2c$ (116, $P\bar{4}c2$); [2] $I\bar{4}2m$ (121)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}2m$ (111)

D_{2d}^3 $P\bar{4}2_1m$ No. 113 $P\bar{4}2_1m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

8	*f*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P21m$ (35, $Cmm2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P22_11$ (18, $P2_12_12$)	1; 2; 5; 6		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$

$P\bar{4}2_1c$ (114)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}2_1c$ (114)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{4}2_1m$ (113)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}2_1m$ (113)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$

[3] $\mathbf{c}'=3\mathbf{c}$

{ $P\bar{4}2_1m$ (113)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{4}2_1m$ (113)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{4}2_1m$ (113)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P\bar{4}2_1m$ (113)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$P\bar{4}2_1m$ (113)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mbm$ (127); [2] $P4/nmm$ (129); [2] $P4_2/mnm$ (136); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C\bar{4}2m$ (115, $P\bar{4}m2$); [2] $I\bar{4}2m$ (121)

- **Decreased unit cell** none

$P\bar{4}2_1c$ No. 114 $P\bar{4}2_1c$ D_{2d}^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P21c$ (37, $Ccc2$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P22_11$ (18, $P2_12_12$)	1; 2; 5; 6		$0,0,1/4$

II Maximal *klassengleiche* subgroups

• Enlarged unit cell

[3] $\mathbf{c}'=3\mathbf{c}$

$P\bar{4}2_1c$ (114)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{4}2_1c$ (114)	$\langle 2;\ 3+(0,0,2);\ 5+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{4}2_1c$ (114)	$\langle 2;\ 3+(0,0,4);\ 5+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

• Series of maximal isomorphic subgroups

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$P\bar{4}2_1c$ (114)	$\langle 2;\ 3+(0,0,2u);\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P\bar{4}2_1c$ (114)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mnc$ (128); [2] $P4/ncc$ (130); [2] $P4_2/mbc$ (135); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

• Additional centring translations

[2] $C\bar{4}2c$ (116, $P\bar{4}c2$); [2] $I\bar{4}2m$ (121)

• Decreased unit cell

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}2_1m$ (113)

D_{2d}^5 $P\bar{4}m2$ No. 115 $P\bar{4}m2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P2m1$ (25, $Pmm2$)	1; 2; 5; 6		
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{4}c2$ (116)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}c2$ (116)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{4}m2$ (115)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}m2$ (115)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C\bar{4}m2_1$ (113, $P\bar{4}2_1m$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}m2_1$ (113, $P\bar{4}2_1m$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C\bar{4}m2$ (111, $P\bar{4}2m$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}m2$ (111, $P\bar{4}2m$)	$\langle 2;\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F\bar{4}m2$ (121, $I\bar{4}2m$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F\bar{4}m2$ (121, $I\bar{4}2m$)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F\bar{4}m2$ (121, $I\bar{4}2m$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F\bar{4}m2$ (121, $I\bar{4}2m$)	$\langle 2;\ 3+(1,0,1);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$\{$ $P\bar{4}m2$ (115)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{4}m2$ (115)	$\langle 2;\ 5;\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{4}m2$ (115)	$\langle 2;\ 5;\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{4}m2$ (115)	$\langle 2;\ 5;\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{4}m2$ (115)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mmm$ (123); [2] $P4/nmm$ (129); [2] $P4_2/mmc$ (131); [2] $P4_2/nmc$ (137)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C\bar{4}m2$ (111, $P\bar{4}2m$); [2] $I\bar{4}m2$ (119)

- **Decreased unit cell** none

$P\bar{4}c2$ No. 116 $P\bar{4}c2$ D_{2d}^{6}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P2c1$ (27, $Pcc2$)	1; 2; 5; 6		
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C\bar{4}c2_1$ (114, $P\bar{4}2_1c$)	$\langle 2;\ 3;\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}c2_1$ (114, $P\bar{4}2_1c$)	$\langle 2;\ 5;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C\bar{4}c2$ (112, $P\bar{4}2c$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C\bar{4}c2$ (112, $P\bar{4}2c$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P\bar{4}c2$ (116)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{4}c2$ (116)	$\langle 2;\ 3+(0,0,2);\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{4}c2$ (116)	$\langle 2;\ 3+(0,0,4);\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P\bar{4}c2$ (116)	$\langle 2;\ 3+(0,0,2u);\ 5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{4}c2$ (116)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/mcc$ (124); [2] $P4/ncc$ (130); [2] $P4_2/mcm$ (132); [2] $P4_2/ncm$ (138)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C\bar{4}c2$ (112, $P\bar{4}2c$); [2] $I\bar{4}c2$ (120)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}m2$ (115)

D_{2d}^{7} $P\bar{4}b2$ No. 117 $P\bar{4}b2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P2b1$ (32, $Pba2$)	1; 2; 5; 6		
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{4}n2$ (118)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}n2$ (118)	$\langle 2;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{4}b2$ (117)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{4}b2$ (117)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{4}b2$ (117)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{4}b2$ (117)	$\langle 2;\ 5;\ 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{4}b2$ (117)	$\langle 2;\ 5;\ 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{4}b2$ (117)	$\langle 2;\ 5;\ 3+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{4}b2$ (117)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/nbm$ (125); [2] $P4/mbm$ (127); [2] $P4_2/nbc$ (133); [2] $P4_2/mbc$ (135)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C\bar{4}m2$ (111, $P\bar{4}2m$); [2] $I\bar{4}c2$ (120)

- **Decreased unit cell** none

$P\bar{4}n2$ No. 118 $P\bar{4}n2$ D_{2d}^{8}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}11$ (81, $P\bar{4}$)	1; 2; 3; 4		
[2] $P2n1$ (34, $Pnn2$)	1; 2; 5; 6		
[2] $P212$ (21, $C222$)	1; 2; 7; 8	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F\bar{4}d2$ (122, $I\bar{4}2d$)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F\bar{4}d2$ (122, $I\bar{4}2d$)	$\langle 2;\ 5;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F\bar{4}d2$ (122, $I\bar{4}2d$)	$\langle 2;\ 3+(1,0,0);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F\bar{4}d2$ (122, $I\bar{4}2d$)	$\langle 2;\ 3+(1,0,1);\ 5+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P\bar{4}n2$ (118)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{4}n2$ (118)	$\langle 2;\ 3+(0,0,2);\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{4}n2$ (118)	$\langle 2;\ 3+(0,0,4);\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P\bar{4}n2$ (118)	$\langle 2;\ 3+(0,0,2u);\ 5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{4}n2$ (118)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P4/nnc$ (126); [2] $P4/mnc$ (128); [2] $P4_2/nnm$ (134); [2] $P4_2/mnm$ (136)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C\bar{4}c2$ (112, $P\bar{4}2c$); [2] $I\bar{4}m2$ (119)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}b2$ (117)

D_{2d}^9 $I\bar{4}m2$ No. 119 $I\bar{4}m2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
16	j	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $y,\bar{x},\bar{z}$ (4) $\bar{y},x,\bar{z}$
			(5) $x,\bar{y},z$ (6) $\bar{x},y,z$ (7) $y,x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}11$ (82, $I\bar{4}$)	(1; 2; 3; 4)+		
[2] $I2m1$ (44, $Imm2$)	(1; 2; 5; 6)+		
[2] $I212$ (22, $F222$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P\bar{4}n2$ (118)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,1/4$
[2] $P\bar{4}m2$ (115)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P\bar{4}m2$ (115)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,1/4$

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I\bar{4}m2$ (119)	$\langle 2; 3; 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I\bar{4}m2$ (119)	$\langle 2; 5; 3+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I\bar{4}m2$ (119)	$\langle 2; 5; 3+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I\bar{4}m2$ (119)	$\langle 2; 5; 3+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$I\bar{4}m2$ (119)	$\langle 2+(2u,2v,0); 3+(u-v,u+v,0); 5+(0,2v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4/mmm$ (139); [2] $I4_1/amd$ (141); [3] $F\bar{4}3m$ (216)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C\bar{4}m2$ (111, $P\bar{4}2m$)

$I\bar{4}c2$ No. 120 $I\bar{4}c2$ D_{2d}^{10}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}11$ (82, $I\bar{4}$)	(1; 2; 3; 4)+		
[2] $I2c1$ (45, $Iba2$)	(1; 2; 5; 6)+		
[2] $I212$ (22, $F222$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P\bar{4}b2$ (117)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,1/4$
[2] $P\bar{4}c2$ (116)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P\bar{4}c2$ (116)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,1/4$

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I\bar{4}c2$ (120)	$\langle 2;\ 3;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I\bar{4}c2$ (120)	$\langle 2;\ 3+(0,0,2);\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I\bar{4}c2$ (120)	$\langle 2;\ 3+(0,0,4);\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$I\bar{4}c2$ (120)	$\langle 2;\ 3+(0,0,2u);\ 5+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$I\bar{4}c2$ (120)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);\ 5+(0,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4/mcm$ (140); [2] $I4_1/acd$ (142); [3] $F\bar{4}3c$ (219)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C\bar{4}m2$ (111, $P\bar{4}2m$)

D_{2d}^{11} $I\bar{4}2m$ No. 121 $I\bar{4}2m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}11$ (82, $I\bar{4}$)	(1; 2; 3; 4)+		
[2] $I21m$ (42, $Fmm2$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $I221$ (23, $I222$)	(1; 2; 5; 6)+		

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P\bar{4}2_1c$ (114)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P\bar{4}2_1m$ (113)	1; 2; 7; 8; (3; 4; 5; 6) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,1/4$
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; (3; 4; 7; 8) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,1/4$
[2] $P\bar{4}2m$ (111)	1; 2; 3; 4; 5; 6; 7; 8		

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I\bar{4}2m$ (121)	$\langle 2;\ 3;\ 5\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I\bar{4}2m$ (121)	$\langle 2;\ (3;\ 5)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I\bar{4}2m$ (121)	$\langle 2;\ (3;\ 5)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I\bar{4}2m$ (121)	$\langle 2;\ (3;\ 5)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$I\bar{4}2m$ (121)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);\ 5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4/mmm$ (139); [2] $I4/mcm$ (140); [3] $I\bar{4}3m$ (217)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C\bar{4}2m$ (115, $P\bar{4}m2$)

$I\bar{4}2d$ No. 122 $I\bar{4}2d$ D_{2d}^{12}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{3}{4}$	(7) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(8) $y+\frac{1}{2},x,z+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}11$ (82, $I\bar{4}$)	(1; 2; 3; 4)+		
[2] $I21d$ (43, $Fdd2$)	(1; 2; 7; 8)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $I221$ (24, $I2_12_12_1$)	(1; 2; 5; 6)+		$0,1/4,3/8$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I\bar{4}2d$ (122)	$\langle 2+(1,0,0);\ 3+(\frac{1}{2},\frac{1}{2},\frac{1}{2});\ 5+(1,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1/4$
$I\bar{4}2d$ (122)	$\langle 2+(1,0,0);\ 3+(\frac{1}{2},\frac{1}{2},\frac{5}{2});\ 5+(1,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,5/4$
$I\bar{4}2d$ (122)	$\langle 2+(1,0,0);\ 3+(\frac{1}{2},\frac{1}{2},\frac{9}{2});\ 5+(1,0,6)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,9/4$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I\bar{4}2d$ (122)	$\langle 2+(1,0,0);\ 3+(\frac{1}{2},\frac{1}{2},\frac{1}{2}+u);$ $5+(1,0,\frac{3p}{4}-\frac{1}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3 \pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,1/4+u$
$I\bar{4}2d$ (122)	$\langle 2;\ 3;\ 5+(0,0,\frac{3p}{4}-\frac{3}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$I\bar{4}2d$ (122)	$\langle 2+(2u,2v,0);\ 3+(u-v,u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $I4_1/amd$ (141); [2] $I4_1/acd$ (142); [3] $I\bar{4}3d$ (220)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C\bar{4}2d$ (118, $P\bar{4}n2$)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 123, pp. 249–250.

D_{4h}^1 $P4/m2/m2/m$ No. 123 $P4/mmm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	u	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4/m11$ (83, $P4/m$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/m12/m$ (65, $Cmmm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/m2/m1$ (47, $Pmmm$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/mcm$ (132)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/mcm$ (132)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_2/mmc$ (131)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/mmc$ (131)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/mcc$ (124)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/mcc$ (124)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/mmm$ (123)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/mmm$ (123)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4/emm$ (129, $P4/nmm$)	$\langle 2;\ 3;\ (5;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4/emm$ (129, $P4/nmm$)	$\langle 2;\ 5;\ (3;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4/mmd$ (127, $P4/mbm$)	$\langle 2;\ 3;\ 9;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4/mmd$ (127, $P4/mbm$)	$\langle 2;\ 5;\ 9;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4/emd$ (125, $P4/nbm$)	$\langle 2;\ 3;\ 5;\ 9+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4/emd$ (125, $P4/nbm$)	$\langle 2;\ (3;\ 5)+(1,0,0);\ 9+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4/mmm$ (123, $P4/mmm$)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4/mmm$ (123, $P4/mmm$)	$\langle (2;\ 9)+(1,1,0);\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F4/mmc$ (140, $I4/mcm$)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4/mmc$ (140, $I4/mcm$)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F4/mmc$ (140, $I4/mcm$)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4/mmc$ (140, $I4/mcm$)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$F4/mmm$ (139, $I4/mmm$)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4/mmm$ (139, $I4/mmm$)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F4/mmm$ (139, $I4/mmm$)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4/mmm$ (139, $I4/mmm$)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4/mmm$ (123)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/mmm$ (123)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/mmm$ (123)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4/mmm$ (123)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/mmm$ (123)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Pm\bar{3}m$ (221)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4/mmm$ (139)

- **Decreased unit cell** none

D_{4h}^2 $P4/m2/c2/c$ No. 124 $P4/mcc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		$0,0,1/4$
[2] $P4/m11$ (83, $P4/m$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/m12/c$ (66, $Cccm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/m2/c1$ (49, $Pccm$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4/ecc$ (130, $P4/ncc$)	$\langle 2;\ 3;\ (5;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4/ecc$ (130, $P4/ncc$)	$\langle 2;\ 5;\ (3;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4/mcd$ (128, $P4/mnc$)	$\langle 2;\ 3;\ 9;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4/mcd$ (128, $P4/mnc$)	$\langle 2;\ 5;\ 9;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4/ecd$ (126, $P4/nnc$)	$\langle 2;\ 3;\ 5;\ 9+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4/ecd$ (126, $P4/nnc$)	$\langle 2;\ (3;\ 5;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4/mcc$ (124, $P4/mcc$)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4/mcc$ (124, $P4/mcc$)	$\langle (2;\ 9)+(1,1,0);\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4/mcc$ (124)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/mcc$ (124)	$\langle 2;\ 3;\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/mcc$ (124)	$\langle 2;\ 3;\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4/mcc$ (124)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/mcc$ (124)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/mmm$ (123)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 125, pp. 252–253.

$P4/nbm$ No. 125 $P4/n2/b2/m$ D_{4h}^{3}

ORIGIN CHOICE 1, Origin at 422 at $4/n22/g$, at $-\frac{1}{4},-\frac{1}{4},0$ from centre $(2/m)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		$0,1/2,0$
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		$0,1/2,0$
[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		$0,1/2,0$
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/4,3/4,0$
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$

$P4_2/nnm$ (134)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$P4_2/nnm$ (134)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$P4_2/nbc$ (133)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$P4_2/nbc$ (133)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$

[3] $\mathbf{c}'=3\mathbf{c}$

$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4/nbm$ (125)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0);$ $9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mcm$ (140)

- **Decreased unit cell** none

D_{4h}^{3} $P4/n2/b2/m$ No. 125 $P4/nbm$

ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $n(b,a)(2_1/g,2/m)$, at $\frac{1}{4},\frac{1}{4},0$ from 422

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
16 n 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$
	(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$
	(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$
	(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		$1/4,3/4,0$
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		$1/4,3/4,0$
[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,1/4,0$
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		$1/4,1/4,0$
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/nnm$ (134)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/nnm$ (134)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_2/nbc$ (133)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/nbc$ (133)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4/nbm$ (125)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P4/nbm$ (125)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)$; $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0)$; $5+(\frac{p}{2}-\frac{1}{2}+2u,0,0)$; $9+(2u,2v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mcm$ (140)

- **Decreased unit cell** none

$P4/nnc$ No. 126 $P4/n2/n2/c$ D_{4h}^{4}

ORIGIN CHOICE 1, Origin at $422/n$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
16 k 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
	(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
	(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
	(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14		$0,1/2,1/4$
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		$0,1/2,1/4$
[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		$0,1/2,1/4$
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/n2/n1$ (48, $Pnnn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4/nnc$ (126)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5+(0,0,2);\ 9+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5+(0,0,4);\ 9+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4/nnc$ (126)	$\langle 2;\ 3;\ 5+(0,0,2u);\ 9+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4/nnc$ (126)	$\langle 2+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(2u,0,0);$ $9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Pn\bar{3}n$ (222)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4/mmm$ (139); [2] $C4/mcc$ (124, $P4/mcc$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nbm$ (125)

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $nn(n,c)$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 422

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	k	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$
			(13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14		$1/4,3/4,0$
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		$1/4,3/4,0$
[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,1/4,0$
[2] $P422$ (89)	1; 2; 3; 4; 5; 6; 7; 8		$1/4,1/4,1/4$
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/n2/n1$ (48, $Pnnn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4/nnc$ (126)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/nnc$ (126)	$\langle 2;\ 3;\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$P4/nnc$ (126)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4/nnc$ (126)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}-2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Pn\bar{3}n$ (222)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4/mmm$ (139); [2] $C4/mcc$ (124, $P4/mcc$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nbm$ (125)

$P4/mbm$ No. 127 $P4/m2_1/b2/m$ D_{4h}^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4bm$ (100)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8		$0,1/2,0$
[2] $P4/m11$ (83, $P4/m$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/m12/m$ (65, $Cmmm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2/m2_1/b1$ (55, $Pbam$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/mnm$ (136)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$P4_2/mnm$ (136)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$P4_2/mbc$ (135)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/mbc$ (135)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/mnc$ (128)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/mnc$ (128)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/mbm$ (127)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/mbm$ (127)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4/mbm$ (127)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/mbm$ (127)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/mbm$ (127)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4/mbm$ (127)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/mbm$ (127)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(p-\frac{1}{2}+2u,p-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mcm$ (140)

- **Decreased unit cell** none

D_{4h}^{6} $P4/m2_1/n2/c$ No. 128 $P4/mnc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4nc$ (104)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8		$0,1/2,1/4$
[2] $P4/m11$ (83, $P4/m$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/m12/c$ (66, $Cccm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2/m2_1/n1$ (58, $Pnnm$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4/mnc$ (128)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/mnc$ (128)	$\langle 2;\ 3;\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/mnc$ (128)	$\langle 2;\ 3;\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4/mnc$ (128)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 9+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4/mnc$ (128)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mcc$ (124, $P4/mcc$); [2] $I4/mmm$ (139)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/mbm$ (127)

$P4/nmm$ No. 129 $P4/n2_1/m2/m$ D_{4h}^7

ORIGIN CHOICE 1, Origin at $\bar{4}m2$ at $\bar{4}/nm2/g$, at $-\frac{1}{4}, \frac{1}{4}, 0$ from centre $(2/m)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16		1/2, 0, 0
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	1/4, 3/4, 0
[2] $P2/n2_1/m1$ (59, $Pmmn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P4_2/ncm$ (138)	$\langle 2; 9; (3; 5) + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	0, 0, −1/2
$P4_2/ncm$ (138)	$\langle 2; 5; (3; 9) + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P4_2/nmc$ (137)	$\langle 2; 5; 9; 3 + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	0, 0, −1/2
$P4_2/nmc$ (137)	$\langle 2; (3; 5; 9) + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P4/ncc$ (130)	$\langle 2; 3; 9; 5 + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P4/ncc$ (130)	$\langle 2; 3; 5; 9 + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
$P4/nmm$ (129)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,1) \rangle$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	0, 0, 1/2
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P4/nmm$ (129)	$\langle 2; 3; 5; 9 \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,2) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 1
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,4) \rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$P4/nmm$ (129)	$\langle 2; 3; (5; 9) + (0,0,2u) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$
$[p^2]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$			
$P4/nmm$ (129)	$\langle 2 + (2u, 2v, 0)$; $3 + (\frac{p}{2} - \frac{1}{2} + u + v, \frac{p}{2} - \frac{1}{2} - u + v, 0)$; $5 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 0)$; $9 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2} + 2v, 0) \rangle$ $p > 2$; $0 \le u < p$; $0 \le v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mmm$ (139)

- **Decreased unit cell** none

D_{4h}^7	$P4/n2_1/m2/m$	No. 129	$P4/nmm$

ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $n2_1$ $(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, 0$ from $\bar{4}m2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	k	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$
			(13) $x,\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		$1/4,3/4,0$
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16		$1/4,3/4,0$
[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,1/4,0$
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8		$1/4,3/4,0$
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/n2_1/m1$ (59, $Pmmn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P4_2/ncm$ (138)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/ncm$ (138)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4_2/nmc$ (137)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4_2/nmc$ (137)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/ncc$ (130)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/ncc$ (130)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P4/nmm$ (129)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P4/nmm$ (129)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4/nmm$ (129)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/nmm$ (129)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4/nmm$ (129)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P4/nmm$ (129)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4/nmm$ (129)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(2u,\frac{p}{2}-\frac{1}{2},0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mmm$ (123, $P4/mmm$); [2] $I4/mmm$ (139)

- **Decreased unit cell** none

$P4/ncc$ No. 130 $P4/n2_1/c2/c$ D_{4h}^8

ORIGIN CHOICE 1, Origin at $\bar{4}/ncn$, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16		0, 1/2, 0
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8		0, 0, 1/4
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	0, 0, 1/4
[2] $P2/n2_1/c1$ (56, $Pccn$)	1; 2; 5; 6; 9; 10; 13; 14		1/4, 1/4, 0

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$P4/ncc$ (130)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/ncc$ (130)	$\langle 2;\ 3;\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$P4/ncc$ (130)	$\langle 2;\ 3;\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$

$P4/ncc$ (130)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$

$P4/ncc$ (130)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0);$ $9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mcc$ (124, $P4/mcc$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P4/nmm$ (129)

D_{4h}^{8} $P4/n2_1/c2/c$ No. 130 $P4/ncc$

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $n1(c,n)$, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$
			(13) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14		1/4, 3/4, 0
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		1/4, 3/4, 0
[2] $P4cc$ (103)	1; 2; 3; 4; 13; 14; 15; 16		1/4, 1/4, 0
[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8		1/4, 3/4, 1/4
[2] $P4/n11$ (85, $P4/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	0, 1/2, 0
[2] $P2/n2_1/c1$ (56, $Pccn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4/ncc$ (130)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4/ncc$ (130)	$\langle 2;\ 3;\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$P4/ncc$ (130)	$\langle 2;\ 3;\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4/ncc$ (130)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4/ncc$ (130)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(2u,\frac{p}{2}-\frac{1}{2},0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4/mcc$ (124, $P4/mcc$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nmm$ (129)

$P4_2/mmc$ No. 131 $P4_2/m2/m2/c$ D_{4h}^9

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	r	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		$0,0,1/4$
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		$0,0,1/4$
[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4_2/m11$ (84, $P4_2/m$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/m12/c$ (66, $Cccm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/m2/m1$ (47, $Pmmm$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$C4_2/emc$ (138, $P4_2/ncm$)	$\langle 2;\ 3;\ (5;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4_2/emc$ (138, $P4_2/ncm$)	$\langle 2;\ 5;\ (3;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4_2/mmd$ (136, $P4_2/mnm$)	$\langle 2;\ 5;\ 9;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2/mmd$ (136, $P4_2/mnm$)	$\langle 2;\ 3;\ 9;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4_2/emd$ (134, $P4_2/nnm$)	$\langle 2;\ 3;\ 5;\ 9+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4_2/emd$ (134, $P4_2/nnm$)	$\langle 2;\ (3;\ 5;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4_2/mmc$ (132, $P4_2/mcm$)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2/mmc$ (132, $P4_2/mcm$)	$\langle 2;\ 9;\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_2/mmc$ (131)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/mmc$ (131)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/mmc$ (131)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P4_2/mmc$ (131)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_2/mmc$ (131)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Pm\bar{3}n$ (223)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mmc$ (132, $P4_2/mcm$); [2] $I4/mmm$ (139)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/mmm$ (123)

D_{4h}^{10} $P4_2/m2/c2/m$ No. 132 $P4_2/mcm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14		$0,0,1/4$
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		$0,0,1/4$
[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8		$0,0,1/4$
[2] $P4_2/m11$ (84, $P4_2/m$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/m12/m$ (65, $Cmmm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/m2/c1$ (49, $Pccm$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
$C4_2/ecm$ (137, $P4_2/nmc$)	$\langle 2;\ 3;\ (5;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4_2/ecm$ (137, $P4_2/nmc$)	$\langle 2;\ 5;\ (3;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4_2/mcd$ (135, $P4_2/mbc$)	$\langle 2;\ 3;\ 9;\ 5+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2/mcd$ (135, $P4_2/mbc$)	$\langle 2;\ 5;\ 9;\ 3+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
$C4_2/ecd$ (133, $P4_2/nbc$)	$\langle 2;\ 3;\ 5;\ 9+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
$C4_2/ecd$ (133, $P4_2/nbc$)	$\langle 2;\ (3;\ 5;\ 9)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
$C4_2/mcm$ (131, $P4_2/mmc$)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
$C4_2/mcm$ (131, $P4_2/mmc$)	$\langle 2;\ 9;\ (3;\ 5)+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,1/2,0$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_2/mcm$ (132)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/mcm$ (132)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/mcm$ (132)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P4_2/mcm$ (132)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P4_2/mcm$ (132)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(2u,0,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mcm$ (131, $P4_2/mmc$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/mmm$ (123)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 133, pp. 264–265.

$P4_2/nbc$ No. 133 $P4_2/n2/b2/c$ D_{4h}^{11}

ORIGIN CHOICE 1, Origin at $\bar{4}12_1/c$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16		$0,1/2,0$
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8		$0,1/2,1/4$
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/2,0,0$
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/nbc$ (133)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/nbc$ (133)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/nbc$ (133)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/nbc$ (133) $\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ (5;\ 9)+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $\mathbf{a},\mathbf{b},p\mathbf{c}$ $0,0,u$

$p>2$; $0\le u<p$

p conjugate subgroups for the prime p

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$P4_2/nbc$ (133) $\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(2u,0,0);\ 9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p\mathbf{a},p\mathbf{b},\mathbf{c}$ $u,v,0$

$p>2$; $0\le u<p$; $0\le v<p$

p^2 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mmc$ (132, $P4_2/mcm$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nbm$ (125)

D_{4h}^{11} $P4_2/n2/b2/c$ No. 133 $P4_2/nbc$

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $n(b,a)(n,c)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	k	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		1/4, 3/4, 1/4
[2] $P\bar{4}2c$ (112)	1; 2; 5; 6; 11; 12; 15; 16		1/4, 3/4, 1/4
[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16		1/4, 1/4, 0
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8		1/4, 1/4, 0
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		0, 1/2, 0
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/n2/b1$ (50, $Pban$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/nbc$ (133)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/nbc$ (133)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$P4_2/nbc$ (133)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/nbc$ (133)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/nbc$ (133)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mmc$ (132, $P4_2/mcm$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nbm$ (125)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 134, pp. 266–267.

$P4_2/nnm$ No. 134 $P4_2/n2/n2/m$ D_{4h}^{12}

ORIGIN CHOICE 1, Origin at $\bar{4}2m$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from centre $(2/m)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8		$0,1/2,0$
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/4,1/4,1/4$
[2] $P2/n2/n1$ (48, $Pnnn$)	1; 2; 5; 6; 9; 10; 13; 14		$1/2,1/2,1/2$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 2;\ 3;\ 5;\ 9+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,0$
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 2;\ 3;\ 5;\ 9\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 2;\ 3;\ (5;\ 9)+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_2/nnm$ (134)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/nnm$ (134)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,2);\ 9+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/nnm$ (134)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,4);\ 9+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P4_2/nnm$ (134)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,2u);$ $9+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_2/nnm$ (134)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(2u,0,0);\ 9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Pn\bar{3}m$ (224)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mcm$ (131, $P4_2/mmc$); [2] $I4/mmm$ (139)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nbm$ (125)

D_{4h}^{12} $P4_2/n2/n2/m$ No. 134 $P4_2/nnm$

ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $nn(2_1/g,2/m)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}2m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
16 n 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$
	(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$
	(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
	(13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14		$1/4,3/4,1/4$
[2] $P\bar{4}2m$ (111)	1; 2; 5; 6; 11; 12; 15; 16		$1/4,3/4,1/4$
[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,3/4,0$
[2] $P4_222$ (93)	1; 2; 3; 4; 5; 6; 7; 8		$1/4,1/4,1/4$
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		$0,1/2,0$
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2/n2/n1$ (48, $Pnnn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 5;\ 2+(1,0,0);\ 3+(0,1,1);\ 9+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 2+(1,0,0);\ (3;\ 9)+(0,1,1);\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 2+(1,0,0);\ (3;\ 9)+(0,1,0);\ 5+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,0,0$
$F4_1/ddc$ (142, $I4_1/acd$)	$\langle 5;\ 2+(1,0,0);\ 3+(0,1,0);\ 9+(0,1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,0,1/2$
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 2+(1,0,0);\ 3+(0,1,1);\ 5+(0,0,1);\ 9+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,1/2,0$
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 5;\ 2+(1,0,0);\ (3;\ 9)+(0,1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,1/2,1/2$
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 5;\ 2+(1,0,0);\ (3;\ 9)+(0,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,0,0$
$F4_1/ddm$ (141, $I4_1/amd$)	$\langle 2+(1,0,0);\ 3+(0,1,0);\ 5+(0,0,1);\ 9+(0,1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$1/2,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P4_2/nnm$ (134)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/nnm$ (134)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/nnm$ (134)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P4_2/nnm$ (134)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P4_2/nnm$ (134)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Pn\bar{3}m$ (224)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mcm$ (131, $P4_2/mmc$); [2] $I4/mmm$ (139)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nbm$ (125)

$P4_2/mbc$ No. 135 $P4_2/m2_1/b2/c$ D_{4h}^{13}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
16 i 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$
	(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
	(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$
	(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}b2$ (117)	1; 2; 7; 8; 11; 12; 13; 14		0,0,1/4
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		0,0,1/4
[2] $P4_2bc$ (106)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8		0,1/2,1/4
[2] $P4_2/m11$ (84, $P4_2/m$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/m12/c$ (66, $Cccm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	0,1/2,0
[2] $P2/m2_1/b1$ (55, $Pbam$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/mbc$ (135)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/mbc$ (135)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,1
$P4_2/mbc$ (135)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0,0,2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/mbc$ (135)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/mbc$ (135)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mmc$ (132, $P4_2/mcm$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/mbm$ (127)

D_{4h}^{14} $P4_2/m2_1/n2/m$ No. 136 $P4_2/mnm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}n2$ (118)	1; 2; 7; 8; 11; 12; 13; 14		$0,1/2,1/4$
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16		$0,1/2,1/4$
[2] $P4_2nm$ (102)	1; 2; 3; 4; 13; 14; 15; 16		
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4_2/m11$ (84, $P4_2/m$)	1; 2; 3; 4; 9; 10; 11; 12		$0,1/2,0$
[2] $P2/m12/m$ (65, $Cmmm$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/m2_1/n1$ (58, $Pnnm$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/mnm$ (136)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/mnm$ (136)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/mnm$ (136)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/mnm$ (136)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/mnm$ (136)	$\langle (2;\ 9)+(2u,2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mcm$ (131, $P4_2/mmc$); [2] $I4/mmm$ (139)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/mbm$ (127)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 137, pp. 270–271.

$P4_2/nmc$ No. 137 $P4_2/n2_1/m2/c$ D_{4h}^{15}

ORIGIN CHOICE 1, Origin at $\bar{4}m2/n$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

16 h 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16		$0,1/2,0$
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8		
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/n2_1/m1$ (59, $Pmmn$)	1; 2; 5; 6; 9; 10; 13; 14		$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/nmc$ (137)	$\langle 2;\ (3;\ 5;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/nmc$ (137)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/nmc$ (137)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/nmc$ (137)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ (5;\ 9)+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/nmc$ (137)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0);$ $9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mmc$ (132, $P4_2/mcm$); [2] $I4/mmm$ (139)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nmm$ (129)

D_{4h}^{15} $P4_2/n2_1/m2/c$ No. 137 $P4_2/nmc$

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $n2_1$ (c,n), at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}m2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(13) $x,\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14		$1/4,3/4,1/4$
[2] $P\bar{4}2_1c$ (114)	1; 2; 5; 6; 11; 12; 15; 16		$1/4,3/4,1/4$
[2] $P4_2mc$ (105)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,1/4,0$
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8		$1/4,3/4,1/4$
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		$0,1/2,0$
[2] $P2/n12/c$ (68, $Ccce$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$
[2] $P2/n2_1/m1$ (59, $Pmmn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/nmc$ (137)	$\langle 2;\ 5;\ 9;\ 3+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/nmc$ (137)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/nmc$ (137)	$\langle 2;\ 3+(0,0,1);\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$P4_2/nmc$ (137)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ (5;\ 9)+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/nmc$ (137)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(2u,\frac{p}{2}-\frac{1}{2},0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mmc$ (132, $P4_2/mcm$); [2] $I4/mmm$ (139)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nmm$ (129)

$P4_2/ncm$ No. 138 $P4_2/n2_1/c2/m$ D_{4h}^{16}

ORIGIN CHOICE 1, Origin at $\bar{4}cg$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from centre $(2/m)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14		
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16		
[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16		$0,1/2,0$
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8		$0,0,1/4$
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/4,3/4,1/4$
[2] $P2/n2_1/c1$ (56, $Pccn$)	1; 2; 5; 6; 9; 10; 13; 14		$1/4,1/4,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/ncm$ (138)	$\langle 2;\ 5;\ (3;\ 9)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/ncm$ (138)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,2);\ 9+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/ncm$ (138)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,4);\ 9+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$P4_2/ncm$ (138)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,2u);$ $9+(0,0,\frac{p}{2}-\frac{1}{2}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/ncm$ (138)	$\langle 2+(2u,2v,0);\ 3+(\frac{p}{2}-\frac{1}{2}+u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},0);$ $9+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mcm$ (131, $P4_2/mmc$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nmm$ (129)

ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $n1\,(2/m,2_1/g)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	j	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(13) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) y,x,z

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}c2$ (116)	1; 2; 7; 8; 11; 12; 13; 14		$1/4,3/4,1/4$
[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16		$1/4,3/4,1/4$
[2] $P4_2cm$ (101)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,1/4,0$
[2] $P4_22_12$ (94)	1; 2; 3; 4; 5; 6; 7; 8		$1/4,3/4,0$
[2] $P4_2/n11$ (86, $P4_2/n$)	1; 2; 3; 4; 9; 10; 11; 12		$0,1/2,0$
[2] $P2/n12/m$ (67, $Cmme$)	1; 2; 7; 8; 9; 10; 15; 16	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
[2] $P2/n2_1/c1$ (56, $Pccn$)	1; 2; 5; 6; 9; 10; 13; 14		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$P4_2/ncm$ (138)	$\langle 2;\ 9;\ (3;\ 5)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P4_2/ncm$ (138)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P4_2/ncm$ (138)	$\langle 2;\ 3+(0,0,1);\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P4_2/ncm$ (138)	$\langle 2;\ 3+(0,0,\frac{p}{2}-\frac{1}{2});\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$P4_2/ncm$ (138)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(\frac{p}{2}-\frac{1}{2}+u+v,-u+v,0);\ 5+(2u,\frac{p}{2}-\frac{1}{2},0);$ $9+(2u,2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $C4_2/mcm$ (131, $P4_2/mmc$); [2] $I4/mcm$ (140)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4/nmm$ (129)

$I4/mmm$ No. 139 $I4/m2/m2/m$ D_{4h}^{17}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
			$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
32	o	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z$	(16) y,x,z

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+		
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+		
[2] $I4mm$ (107)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+		
[2] $I4/m11$ (87, $I4/m$)	(1; 2; 3; 4; 9; 10; 11; 12)+		
[2] $I2/m2/m1$ (71, $Immm$)	(1; 2; 5; 6; 9; 10; 13; 14)+		
[2] $I2/m12/m$ (69, $Fmmm$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2/nmc$ (137)	1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 3/4, 1/4
[2] $P4_2/mnm$ (136)	1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4_2/nnm$ (134)	1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 3/4, 1/4
[2] $P4_2/mmc$ (131)	1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		0, 1/2, 0
[2] $P4/nmm$ (129)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $P4/mnc$ (128)	1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4/nnc$ (126)	1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		1/4, 1/4, 1/4
[2] $P4/mmm$ (123)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16		

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4/mmm$ (139)	$\langle 2;\ 3;\ 5;\ 9 \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9) + (0,0,2) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 1
$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9) + (0,0,4) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	0, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I4/mmm$ (139)	$\langle 2;\ 3;\ (5;\ 9) + (0,0,2u) \rangle$ $p > 2$; $0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$I4/mmm$ (139)	$\langle (2;\ 9) + (2u,2v,0);\ 3 + (u+v,-u+v,0);\ 5 + (2u,0,0) \rangle$ $p > 2$; $0 \le u < p$; $0 \le v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fm\bar{3}m$ (225); [3] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4/mmm$ (123, $P4/mmm$)

D_{4h}^{18} $\quad I4/m2/c2/m$ $\quad$ No. 140 $\quad I4/mcm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	$(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
32 $\quad m\quad$ 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
	(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
	(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$
	(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2m$ (121)	(1; 2; 5; 6; 11; 12; 15; 16)+		$0,1/2,1/4$
[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+		
[2] $I4cm$ (108)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[2] $I422$ (97)	(1; 2; 3; 4; 5; 6; 7; 8)+		$0,0,1/4$
[2] $I4/m11$ (87, $I4/m$)	(1; 2; 3; 4; 9; 10; 11; 12)+		
[2] $I2/m2/c1$ (72, $Ibam$)	(1; 2; 5; 6; 9; 10; 13; 14)+		
[2] $I2/m12/m$ (69, $Fmmm$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,0$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_2/ncm$ (138)	1; 2; 7; 8; 11; 12; 13; 14; (3; 4; 5; 6; 9; 10; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,3/4,1/4$
[2] $P4_2/mbc$ (135)	1; 2; 7; 8; 9; 10; 15; 16; (3; 4; 5; 6; 11; 12; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4_2/nbc$ (133)	1; 2; 5; 6; 11; 12; 15; 16; (3; 4; 7; 8; 9; 10; 13; 14) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,3/4,1/4$
[2] $P4_2/mcm$ (132)	1; 2; 5; 6; 9; 10; 13; 14; (3; 4; 7; 8; 11; 12; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$0,1/2,0$
[2] $P4/ncc$ (130)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $P4/mbm$ (127)	1; 2; 3; 4; 9; 10; 11; 12; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		
[2] $P4/nbm$ (125)	1; 2; 3; 4; 5; 6; 7; 8; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		$1/4,1/4,1/4$
[2] $P4/mcc$ (124)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16		

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$I4/mcm$ (140)	$\langle 2;\ 3;\ 9;\ 5+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$I4/mcm$ (140)	$\langle 2;\ 3;\ 5+(0,0,3);\ 9+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$I4/mcm$ (140)	$\langle 2;\ 3;\ 5+(0,0,5);\ 9+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$I4/mcm$ (140)	$\langle 2;\ 3;\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 9+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$I4/mcm$ (140)	$\langle (2;\ 9)+(2u,2v,0);\ 3+(u+v,-u+v,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0)\rangle$ $p>2;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fm\bar{3}c$ (226)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4/mmm$ (123, $P4/mmm$)

$I4_1/amd$ No. 141 $I4_1/a2/m2/d$ D_{4h}^{19}

ORIGIN CHOICE 1, Origin at $\bar{4}m2$, at $0, \frac{1}{4}, -\frac{1}{8}$ from centre $(2/m)$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

32	*i*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(16) $y,x+\frac{1}{2},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+		
[2] $I4_1md$ (109)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+		
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		
[2] $I2/a2/m1$ (74, $Imma$)	(1; 2; 5; 6; 9; 10; 13; 14)+		$0,1/4,1/8$
[2] $I2/a12/d$ (70, $Fddd$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,1/2,1/4$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4_1/amd$ (141)	$\langle(2;\,9)+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1/4$
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,4);\ 9+(1,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,5/4$
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,6);\ 9+(1,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,9/4$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I4_1/amd$ (141)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});\ 5+(1,0,\frac{3p}{4}-\frac{1}{4}+2u);$ $9+(1,0,\frac{p}{4}+\frac{1}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,1/4+u$
$I4_1/amd$ (141)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});\ 5+(0,0,\frac{3p}{4}-\frac{3}{4}+2u);$ $9+(0,0,\frac{p}{4}-\frac{1}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$

$I4_1/amd$ (141)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);\ 3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 9+(2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fd\bar{3}m$ (227)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4_2/emd$ (134, $P4_2/nnm$)

D_{4h}^{19} $\quad I4_1/a2/m2/d$ $\quad$ No. 141 $\quad I4_1/amd$

ORIGIN CHOICE 2, Origin at centre $(2/m)$ at $b\,(2/m, 2_1/n)\,d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$

Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
32	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	(4) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}$	(7) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	(8) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(11) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$
			(13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $y+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		0, 1/4, 3/8
[2] $I\bar{4}m2$ (119)	(1; 2; 7; 8; 11; 12; 13; 14)+		0, 1/4, 3/8
[2] $I4_1md$ (109)	(1; 2; 3; 4; 13; 14; 15; 16)+		0, 1/4, 0
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+		0, 1/4, 3/8
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		0, 1/2, 0
[2] $I2/a2/m1$ (74, $Imma$)	(1; 2; 5; 6; 9; 10; 13; 14)+		
[2] $I2/a12/d$ (70, $Fddd$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	1/4, 3/4, 1/4

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** $\quad$ none

- **Enlarged unit cell**

[3] $\mathbf{c}' = 3\mathbf{c}$

$I4_1/amd$ (141)	$\langle(2;\ 5)+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 9+(1,0,0)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	1/2, 0, 0
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,3);\ 9+(1,0,2)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	1/2, 0, 1
$I4_1/amd$ (141)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ 5+(1,0,5);\ 9+(1,0,4)\rangle$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	1/2, 0, 2

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$I4_1/amd$ (141)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});\ 5+(1,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(1,0,2u)\rangle$ $p>2;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 3$ (mod 4)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$1/2, 0, u$
$I4_1/amd$ (141)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});\ 5+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $9+(0,0,2u)\rangle$ $p>4;\ 0 \le u < p$ p conjugate subgroups for prime $p \equiv 1$ (mod 4)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0, 0, u$

[p^2] $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$

$I4_1/amd$ (141)	$\langle 2+(\frac{p}{2}+\frac{1}{2}+2u, 2v, 0);\ 3+(\frac{p}{4}+\frac{1}{4}+u+v, \frac{3p}{4}-\frac{5}{4}-u+v, 0);$ $5+(\frac{p}{2}+\frac{1}{2}+2u, 0, 0);\ 9+(1+2u, 2v, 0)\rangle$ $p>2;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 3$ (mod 4)	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$1/2+u, v, 0$
$I4_1/amd$ (141)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u, 2v, 0);\ 3+(\frac{p}{4}-\frac{1}{4}+u+v, \frac{3p}{4}-\frac{3}{4}-u+v, 0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u, 0, 0);\ 9+(2u, 2v, 0)\rangle$ $p>4;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 1$ (mod 4)	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u, v, 0$

I Minimal *translationengleiche* supergroups

[3] $Fd\bar{3}m$ (227)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** $\quad$ none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $C4_2/emd$ (134, $P4_2/nnm$)

$I4_1/acd$ No. 142 $I4_1/a2/c2/d$ D_{4h}^{20}

ORIGIN CHOICE 1, Origin at $\bar{4}c2_1$, at $0, \frac{1}{4}, -\frac{1}{8}$ from $\bar{1}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

32	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{3}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$
			(9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{4}$	(16) $y,x+\frac{1}{2},z+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		$0,1/2,1/4$
[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+		
[2] $I4_1cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+		$0,0,1/4$
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		
[2] $I2/a2/c1$ (73, $Ibca$)	(1; 2; 5; 6; 9; 10; 13; 14)+		$0,1/4,1/8$
[2] $I2/a12/d$ (70, $Fddd$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_1/acd$ (142)	$\langle(2;\ 5;\ 9)+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2})\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1/4$
$I4_1/acd$ (142)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ (5;\ 9)+(1,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,5/4$
$I4_1/acd$ (142)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ (5;\ 9)+(1,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,9/4$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1/acd$ (142)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});$ $(5;\ 9)+(1,0,\frac{p}{4}+\frac{1}{4}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,1/4+u$
$I4_1/acd$ (142)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});$ $(5;\ 9)+(0,0,\frac{p}{4}-\frac{1}{4}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$I4_1/acd$ (142)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $3+(u+v,\frac{p}{2}-\frac{1}{2}-u+v,0);\ 5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);$ $9+(2u,\frac{p}{2}-\frac{1}{2}+2v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fd\bar{3}c$ (228); [3] $Ia\bar{3}d$ (230)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2/emd$ (134, $P4_2/nnm$)

D_{4h}^{20}	$I4_1/a2/c2/d$	No. 142	$I4_1/acd$

ORIGIN CHOICE 2, Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

32	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	(4) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{3}{4}$	(8) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(11) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{4}$	(16) $y+\frac{3}{4},x+\frac{3}{4},z+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}2d$ (122)	(1; 2; 5; 6; 11; 12; 15; 16)+		$0,3/4,1/8$
[2] $I\bar{4}c2$ (120)	(1; 2; 7; 8; 11; 12; 13; 14)+		$0,1/4,3/8$
[2] $I4_1cd$ (110)	(1; 2; 3; 4; 13; 14; 15; 16)+		$0,1/4,0$
[2] $I4_122$ (98)	(1; 2; 3; 4; 5; 6; 7; 8)+		$0,1/4,1/8$
[2] $I4_1/a11$ (88, $I4_1/a$)	(1; 2; 3; 4; 9; 10; 11; 12)+		$0,1/2,0$
[2] $I2/a2/c1$ (73, $Ibca$)	(1; 2; 5; 6; 9; 10; 13; 14)+		
[2] $I2/a12/d$ (70, $Fddd$)	(1; 2; 7; 8; 9; 10; 15; 16)+	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$1/4,1/4,1/4$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$

$I4_1/acd$ (142)	$\langle 5;\ 9;\ 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2})\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,0$
$I4_1/acd$ (142)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ (5;\ 9)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,1$
$I4_1/acd$ (142)	$\langle 2+(1,0,1);\ 3+(\frac{1}{2},-\frac{1}{2},\frac{1}{2});\ (5;\ 9)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$1/2,0,2$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$I4_1/acd$ (142)	$\langle 2+(1,0,\frac{p}{2}-\frac{1}{2});\ 3+(\frac{1}{2},-\frac{1}{2},\frac{p}{4}-\frac{1}{4});\ (5;\ 9)+(1,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 3$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$1/2,0,u$
$I4_1/acd$ (142)	$\langle 2+(0,0,\frac{p}{2}-\frac{1}{2});\ 3+(0,0,\frac{p}{4}-\frac{1}{4});\ (5;\ 9)+(0,0,2u)\rangle$ $p>4;\ 0\leq u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 4)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$I4_1/acd$ (142)	$\langle 2+(\frac{p}{2}+\frac{1}{2}+2u,2v,0);\ 3+(\frac{p}{4}+\frac{1}{4}+u+v,\frac{3p}{4}+\frac{5}{4}-u+v,0);$ $5+(\frac{p}{2}+\frac{1}{2}+2u,0,0);\ 9+(1+2u,2v,0)\rangle$ $p>2;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for prime $p\equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$1/2+u,v,0$
$I4_1/acd$ (142)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,0);\ 3+(\frac{p}{4}-\frac{1}{4}+u+v,\frac{3p}{4}-\frac{3}{4}-u+v,0);$ $5+(\frac{p}{2}-\frac{1}{2}+2u,0,0);\ 9+(2u,2v,0)\rangle$ $p>4;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for prime $p\equiv 1$ (mod 4)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[3] $Fd\bar{3}c$ (228); [3] $Ia\bar{3}d$ (230)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $C4_2/emd$ (134, $P4_2/nnm$)

$P3$ No. 143 $P3$ C_3^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
3	d	1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$

I Maximal *translationengleiche* subgroups

[3] $P1$ (1)	1		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P3$ (143)	$\langle 2 \rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P3_2$ (145)	$\langle 2+(0,0,2) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P3_1$ (144)	$\langle 2+(0,0,1) \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P3$ (143)	$\langle 2 \rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b}$			
$H3$ (143, $P3$)	$\langle 2 \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3$ (143, $P3$)	$\langle 2+(1,0,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3$ (143, $P3$)	$\langle 2+(1,1,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
[3] $\mathbf{a}' = \mathbf{a}-\mathbf{b},\ \mathbf{b}' = \mathbf{a}+2\mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$			
$R3$ (146)	$\langle 2 \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	
$R3$ (146)	$\langle 2+(1,0,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$2/3,1/3,0$
$R3$ (146)	$\langle 2+(1,1,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$1/3,2/3,0$
[3] $\mathbf{a}' = 2\mathbf{a}+\mathbf{b},\ \mathbf{b}' = -\mathbf{a}+\mathbf{b},\ \mathbf{c}' = 3\mathbf{c}$			
$R3$ (146)	$\langle 2 \rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	
$R3$ (146)	$\langle 2+(1,0,0) \rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$2/3,1/3,0$
$R3$ (146)	$\langle 2+(1,1,0) \rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$1/3,2/3,0$
[4] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$P3$ (143)	$\langle 2 \rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3$ (143)	$\langle 2+(1,-1,0) \rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3$ (143)	$\langle 2+(1,2,0) \rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3$ (143)	$\langle 2+(2,1,0) \rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P3$ (143)	$\langle 2 \rangle$ $p > 1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P3$ (143)	$\langle 2+(u+v,-u+2v,0) \rangle$ $p > 1$; $0 \le u < p$; $0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p = q^2+r^2+qr$] $\mathbf{a}' = q\mathbf{a}-r\mathbf{b},\ \mathbf{b}' = r\mathbf{a}+(q+r)\mathbf{b}$			
$P3$ (143)	$\langle 2+(u,-u,0) \rangle$ $q > 0$; $r > 0$; $p > 6$; $p \equiv 1 \pmod 3$; $0 \le u < p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}$ (147); [2] $P312$ (149); [2] $P321$ (150); [2] $P3m1$ (156); [2] $P31m$ (157); [2] $P3c1$ (158); [2] $P31c$ (159); [2] $P6$ (168); [2] $P6_3$ (173); [2] $P\bar{6}$ (174)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $R_{obv}3$ (146, $R3$); [3] $R_{rev}3$ (146, $R3$)

- **Decreased unit cell** none

C_3^2 $P3_1$ No. 144 $P3_1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
3	a	1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{1}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$

I Maximal *translationengleiche* subgroups

[3] $P1$ (1) 1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3_2$ (145)	$\langle 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=3\mathbf{b}$			
$H3_1$ (144, $P3_1$)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3_1$ (144, $P3_1$)	$\langle 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3_1$ (144, $P3_1$)	$\langle 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
{ $P3_1$ (144)	$\langle 2\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P3_1$ (144)	$\langle 2+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P3_1$ (144)	$\langle 2+(1,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P3_1$ (144)	$\langle 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P3_2$ (145)	$\langle 2+(0,0,\frac{2p}{3}-\frac{1}{3})\rangle$ $p>1$; $p\equiv 2 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P3_1$ (144)	$\langle 2+(0,0,\frac{p}{3}-\frac{1}{3})\rangle$ $p>6$; $p\equiv 1 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P3_1$ (144)	$\langle 2+(u+v,-u+2v,0)\rangle$ $p>1$; $p\equiv 2 \pmod 3$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2+qr$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P3_1$ (144)	$\langle 2+(u,-u,0)\rangle$ $q>0$; $r>0$; $p>6$; $0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P3_112$ (151); [2] $P3_121$ (152); [2] $P6_1$ (169); [2] $P6_4$ (172)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $R_{obv}3$ (146, $R3$); [3] $R_{rev}3$ (146, $R3$)

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P3$ (143)

$P3_2$ No. 145 $P3_2$ C_3^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
3	a	1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{2}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$

I Maximal *translationengleiche* subgroups

[3] $P1$ (1) 1

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3_1$ (144)	$\langle 2\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3_2$ (145, $P3_2$)	$\langle 2\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3_2$ (145, $P3_2$)	$\langle 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3_2$ (145, $P3_2$)	$\langle 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3_2$ (145)	$\langle 2\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3_2$ (145)	$\langle 2+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3_2$ (145)	$\langle 2+(1,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3_2$ (145)	$\langle 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P3_2$ (145)	$\langle 2+(0,0,\frac{2p}{3}-\frac{2}{3})\rangle$ $p>6;\ p\equiv 1 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P3_1$ (144)	$\langle 2+(0,0,\frac{p}{3}-\frac{2}{3})\rangle$ $p>1;\ p\equiv 2 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3_2$ (145)	$\langle 2+(u+v,-u+2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2+qr$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P3_2$ (145)	$\langle 2+(u,-u,0)\rangle$ $q>0;\ r>0;\ p>6;\ p\equiv 1 \pmod 3);\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P3_212$ (153); [2] $P3_221$ (154); [2] $P6_5$ (170); [2] $P6_2$ (171)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $R_{obv}3$ (146, $R3$); [3] $R_{rev}3$ (146, $R3$)

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P3$ (143)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 146, pp. 283–284.

C_3^4 $R3$ No. 146 $R3$

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
9 b 1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$

I Maximal *translationengleiche* subgroups

[3] $R1$ (1, $P1$)	1+	$\mathbf{a},\mathbf{b},1/3(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[3] $P3_2$ (145)	1; $2+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; $3+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		$0,1/3,0$
[3] $P3_1$ (144)	1; $2+(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $3+(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		$1/3,1/3,0$
[3] $P3$ (143)	1; 2; 3		

- **Enlarged unit cell**

[2] $\mathbf{a}'=-\mathbf{b}$, $\mathbf{b}'=\mathbf{a}+\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$R3$ (146)	$\langle 2\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$			
{ $R3$ (146)	$\langle 2\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $R3$ (146)	$\langle 2+(1,-1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $R3$ (146)	$\langle 2+(1,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $R3$ (146)	$\langle 2+(2,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$R3$ (146)	$\langle 2\rangle$ $p>1$; $p\equiv 2 \pmod 3$ no conjugate subgroups	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	
$R3$ (146)	$\langle 2\rangle$ $p>6$; $p\equiv 1 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=-p\mathbf{b}$, $\mathbf{b}'=p\mathbf{a}+p\mathbf{b}$			
$R3$ (146)	$\langle 2+(u+v,-u+2v,0)\rangle$ $p>1$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2-qr]$ $\mathbf{a}'=(q-r)\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$R3$ (146)	$\langle 2+(u,-u,0)\rangle$ $q>0$; $r>0$; $q\neq r$; $q+r\equiv 1 \pmod 3$; $p>6$; $0\le u<p$ p conjugate subgroups for each pair of q and r	$(q-r)\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198); [4] $I2_13$ (199)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$, $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$, $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P3$ (143)

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
3	b	1	(1) x,y,z (2) z,x,y (3) y,z,x

I Maximal *translationengleiche* subgroups

[3] $R1$ (1, $P1$) 1

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[2] $\mathbf{a}' = \mathbf{a}+\mathbf{c},\ \mathbf{b}' = \mathbf{a}+\mathbf{b},\ \mathbf{c}' = \mathbf{b}+\mathbf{c}$

$R3$ (146)	$\langle 2 \rangle$	$\mathbf{a}+\mathbf{c},\mathbf{a}+\mathbf{b},\mathbf{b}+\mathbf{c}$	

[3] $\mathbf{a}' = \mathbf{a}-\mathbf{b},\ \mathbf{b}' = \mathbf{b}-\mathbf{c},\ \mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$

$P3_2$ (145)	$\langle 2+(1,1,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0,1/3,-1/3$
$P3_1$ (144)	$\langle 2+(1,0,0) \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/3,0,-1/3$
$P3$ (143)	$\langle 2 \rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	

[4] $\mathbf{a}' = \mathbf{a}-\mathbf{b}+\mathbf{c},\ \mathbf{b}' = \mathbf{a}+\mathbf{b}-\mathbf{c},\ \mathbf{c}' = -\mathbf{a}+\mathbf{b}+\mathbf{c}$

$R3$ (146)	$\langle 2 \rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	
$R3$ (146)	$\langle 2+(1,-2,1) \rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,-1,0$
$R3$ (146)	$\langle 2+(1,1,-2) \rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0,1,-1$
$R3$ (146)	$\langle 2+(2,-1,-1) \rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,-1$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}+(p-2)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}' = \frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(p-2)\mathbf{c}\big),\ \mathbf{c}' = \frac{1}{3}\big((p-2)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R3$ (146) $\langle 2 \rangle$ $\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
$p > 1$; $p \equiv 2 \pmod 3$
no conjugate subgroups

[p] $\mathbf{a}' = \frac{1}{3}\big((p+2)\mathbf{a}+(p-1)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{b}' = \frac{1}{3}\big((p-1)\mathbf{a}+(p+2)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{c}' = \frac{1}{3}\big((p-1)\mathbf{a}+(p-1)\mathbf{b}+(p+2)\mathbf{c}\big)$

$R3$ (146) $\langle 2 \rangle$ $\mathbf{a}' = \frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations
$p > 6$; $p \equiv 1 \pmod 3$
no conjugate subgroups

[p^2] $\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}' = \frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big),\ \mathbf{c}' = \frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R3$ (146) $\langle 2+(u+v,-2u+v,u-2v) \rangle$ $\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
$p > 1$; $0 \le u < p$; $0 \le v < p$ $u,-u+v,-v$
p^2 conjugate subgroups for prime $p \equiv 2 \pmod 3$

[$p = q^2+r^2-qr$] $\mathbf{a}' = \frac{1}{3}(\alpha\mathbf{a}+\beta\mathbf{b}+\gamma\mathbf{c}),\ \mathbf{b}' = \frac{1}{3}(\gamma\mathbf{a}+\alpha\mathbf{b}+\beta\mathbf{c}),\ \mathbf{c}' = \frac{1}{3}(\beta\mathbf{a}+\gamma\mathbf{b}+\alpha\mathbf{c})$; $\alpha = 2q-r+1,\ \beta = 1-q-r,\ \gamma = 2r+1-q$

$R3$ (146) $\langle 2+(u,-2u,u) \rangle$ $\mathbf{a}' = \frac{1}{3}(\alpha\mathbf{a}+\beta\mathbf{b}\ldots$, see lattice relations
$q > 0$; $r > 0$; $q \neq r$; $q+r \equiv 1 \pmod 3$; $p > 6$; $u,-u,0$
$0 \le u < p$
p conjugate subgroups for each pair of q and r

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}$ (148); [2] $R32$ (155); [2] $R3m$ (160); [2] $R3c$ (161); [4] $P23$ (195); [4] $F23$ (196); [4] $I23$ (197); [4] $P2_13$ (198); [4] $I2_13$ (199)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\ \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\ \mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ $P3$ (143)

C_{3i}^1 $P\bar{3}$ No. 147 $P\bar{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},\bar{z}$	(5) $y,\bar{x}+y,\bar{z}$	(6) $x-y,x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P3$ (143)	1; 2; 3
[3] $P\bar{1}$ (2)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{3}$ (147)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{3}$ (147)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P\bar{3}$ (147)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{3}$ (147)	$\langle 2;\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{3}$ (147)	$\langle 2;\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H\bar{3}$ (147, $P\bar{3}$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H\bar{3}$ (147, $P\bar{3}$)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H\bar{3}$ (147, $P\bar{3}$)	$\langle 2+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{a}+2\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R\bar{3}$ (148)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	
$R\bar{3}$ (148)	$\langle 2;\ 4+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,1$
$R\bar{3}$ (148)	$\langle 2;\ 4+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=2\mathbf{a}+\mathbf{b},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R\bar{3}$ (148)	$\langle 2;\ 4\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	
$R\bar{3}$ (148)	$\langle 2;\ 4+(0,0,2)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,1$
$R\bar{3}$ (148)	$\langle 2;\ 4+(0,0,4)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,2$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P\bar{3}$ (147)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P\bar{3}$ (147)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{3}$ (147)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P\bar{3}$ (147)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P\bar{3}$ (147)	$\langle 2;\ 4+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{3}$ (147)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2+qr]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P\bar{3}$ (147)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}1m$ (162); [2] $P\bar{3}1c$ (163); [2] $P\bar{3}m1$ (164); [2] $P\bar{3}c1$ (165); [2] $P6/m$ (175); [2] $P6_3/m$ (176)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $R_{\mathrm{obv}}\bar{3}$ (148, $R\bar{3}$); [3] $R_{\mathrm{rev}}\bar{3}$ (148, $R\bar{3}$)

- **Decreased unit cell** none

$R\bar{3}$ No. 148 $R\bar{3}$ C_{3i}^2

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
	$(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
18 *f* 1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$ (4) $\bar{x},\bar{y},\bar{z}$ (5) $y,\bar{x}+y,\bar{z}$ (6) $x-y,x,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $R3$ (146)	(1; 2; 3)+		
[3] $R\bar{1}$ (2, $P\bar{1}$)	(1; 4)+	$\mathbf{a},\mathbf{b},1/3(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[3] $P\bar{3}$ (147)	1; 2; 3; 4; 5; 6		
[3] $P\bar{3}$ (147)	1; 2; 3; (4; 5; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		2/3, 1/3, 1/3
[3] $P\bar{3}$ (147)	1; 2; 3; (4; 5; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		1/3, 2/3, 2/3

- **Enlarged unit cell**

[2] $\mathbf{a}'=-\mathbf{b}$, $\mathbf{b}'=\mathbf{a}+\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$R\bar{3}$ (148)	$\langle 2;\ 4\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$R\bar{3}$ (148)	$\langle 2;\ 4+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	0, 0, 1/2
[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$			
$R\bar{3}$ (148)	$\langle 2;\ 4\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$R\bar{3}$ (148)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	1, 0, 0
$R\bar{3}$ (148)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	0, 1, 0
$R\bar{3}$ (148)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	1, 1, 0

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$R\bar{3}$ (148)	$\langle 2;\ 4+(0,0,2u)\rangle$ $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 2$ (mod 3)	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	$0,0,u$
$R\bar{3}$ (148)	$\langle 2;\ 4+(0,0,2u)\rangle$ $p>6$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=-p\mathbf{b}$, $\mathbf{b}'=p\mathbf{a}+p\mathbf{b}$			
$R\bar{3}$ (148)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1$; $p\equiv 2$ (mod 3); $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2-qr$] $\mathbf{a}'=(q-r)\mathbf{a}-r\mathbf{b}$, $\mathbf{b}'=r\mathbf{a}+q\mathbf{b}$			
$R\bar{3}$ (148)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0$; $r>0$; $q\neq r$; $q+r\equiv 1$ (mod 3); $p>6$; $0\le u<p$ p conjugate subgroups for each pair of q and r	$(q-r)\mathbf{a}-r\mathbf{b},r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $Pm\bar{3}$ (200); [4] $Pn\bar{3}$ (201); [4] $Fm\bar{3}$ (202); [4] $Fd\bar{3}$ (203); [4] $Im\bar{3}$ (204); [4] $Pa\bar{3}$ (205); [4] $Ia\bar{3}$ (206)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$, $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$, $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P\bar{3}$ (147)

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
6	f	1	(1) x,y,z (2) z,x,y (3) y,z,x (4) $\bar{x},\bar{y},\bar{z}$ (5) $\bar{z},\bar{x},\bar{y}$ (6) $\bar{y},\bar{z},\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $R3$ (146) 1; 2; 3
[3] $R\bar{1}$ (2, $P\bar{1}$) 1; 4

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[2] $\mathbf{a}' = \mathbf{a}+\mathbf{c}$, $\mathbf{b}' = \mathbf{a}+\mathbf{b}$, $\mathbf{c}' = \mathbf{b}+\mathbf{c}$

$R\bar{3}$ (148)	$\langle 2;\ 4\rangle$	$\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}$	
$R\bar{3}$ (148)	$\langle 2;\ 4+(1,1,1)\rangle$	$\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}$	$1/2, 1/2, 1/2$

[3] $\mathbf{a}' = \mathbf{a}-\mathbf{b}$, $\mathbf{b}' = \mathbf{b}-\mathbf{c}$, $\mathbf{c}' = \mathbf{a}+\mathbf{b}+\mathbf{c}$

$P\bar{3}$ (147)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	
$P\bar{3}$ (147)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,0$
$P\bar{3}$ (147)	$\langle 2+(1,0,-1);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,1,0$

[4] $\mathbf{a}' = \mathbf{a}-\mathbf{b}+\mathbf{c}$, $\mathbf{b}' = \mathbf{a}+\mathbf{b}-\mathbf{c}$, $\mathbf{c}' = -\mathbf{a}+\mathbf{b}+\mathbf{c}$

$R\bar{3}$ (148)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	
$R\bar{3}$ (148)	$\langle 2+(1,-2,1);\ 4+(2,-2,0)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,-1,0$
$R\bar{3}$ (148)	$\langle 2+(1,1,-2);\ 4+(0,2,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0,1,-1$
$R\bar{3}$ (148)	$\langle 2+(2,-1,-1);\ 4+(2,0,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,-1$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}+(p-2)\mathbf{b}+(p+1)\mathbf{c}\big)$, $\mathbf{b}' = \frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(p-2)\mathbf{c}\big)$, $\mathbf{c}' = \frac{1}{3}\big((p-2)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R\bar{3}$ (148)	$\langle 2;\ 4+(2u,2u,2u)\rangle$ $p>4$; $0 \le u < p$ p conjugate subgroups for prime $p \equiv 2 \pmod 3$	$\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations	u,u,u

[p] $\mathbf{a}' = \frac{1}{3}\big((p+2)\mathbf{a}+(p-1)\mathbf{b}+(p-1)\mathbf{c}\big)$, $\mathbf{b}' = \frac{1}{3}\big((p-1)\mathbf{a}+(p+2)\mathbf{b}+(p-1)\mathbf{c}\big)$, $\mathbf{c}' = \frac{1}{3}\big((p-1)\mathbf{a}+(p-1)\mathbf{b}+(p+2)\mathbf{c}\big)$

$R\bar{3}$ (148)	$\langle 2;\ 4+(2u,2u,2u)\rangle$ $p>6$; $0 \le u < p$ p conjugate subgroups for prime $p \equiv 1 \pmod 3$	$\mathbf{a}' = \frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations	u,u,u

[p^2] $\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big)$, $\mathbf{b}' = \frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big)$, $\mathbf{c}' = \frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R\bar{3}$ (148)	$\langle 2+(u+v,-2u+v,u-2v)$; $4+(2u,-2u+2v,-2v)\rangle$ $p>1$; $0 \le u < p$; $0 \le v < p$ p^2 conjugate subgroups for prime $p \equiv 2 \pmod 3$	$\mathbf{a}' = \frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations	$u,-u+v,-v$

[$p = q^2+r^2-qr$] $\mathbf{a}' = \frac{1}{3}(\alpha\mathbf{a}+\beta\mathbf{b}+\gamma\mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(\gamma\mathbf{a}+\alpha\mathbf{b}+\beta\mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(\beta\mathbf{a}+\gamma\mathbf{b}+\alpha\mathbf{c})$; $\alpha = 2q-r+1$, $\beta = 1-q-r$, $\gamma = 2r+1-q$

$R\bar{3}$ (148)	$\langle 2+(u,-2u,u);\ 4+(2u,-2u,0)\rangle$ $q>0$; $r>0$; $q \ne r$; $q+r \equiv 1 \pmod 3$; $p>6$; $0 \le u < p$ p conjugate subgroups for each pair of q and r	$\mathbf{a}' = \frac{1}{3}(\alpha\mathbf{a}+\beta\mathbf{b}+\ldots$, see lattice relations	$u,-u,0$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $Pm\bar{3}$ (200); [4] $Pn\bar{3}$ (201); [4] $Fm\bar{3}$ (202); [4] $Fd\bar{3}$ (203); [4] $Im\bar{3}$ (204); [4] $Pa\bar{3}$ (205); [4] $Ia\bar{3}$ (206)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ $P\bar{3}$ (147)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 149, pp. 288–289.

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},\bar{z}$	(5) $\bar{x}+y,y,\bar{z}$	(6) $x,x-y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P311$ (143, $P3$)	1; 2; 3		
[3] $P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P112$ (5, $C121$)	1; 5	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
[3] $P112$ (5, $C121$)	1; 6	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P312$ (149)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P312$ (149)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P3_212$ (153)	$\langle 2+(0,0,2);\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P3_212$ (153)	$\langle 2+(0,0,2);\ 4+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P3_212$ (153)	$\langle 2+(0,0,2);\ 4+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
$P3_112$ (151)	$\langle 2+(0,0,1);\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P3_112$ (151)	$\langle 2+(0,0,1);\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P3_112$ (151)	$\langle 2+(0,0,1);\ 4+(0,0,6)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
$P312$ (149)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P312$ (149)	$\langle 2;\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P312$ (149)	$\langle 2;\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H312$ (150, $P321$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H312$ (150, $P321$)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H312$ (150, $P321$)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H312$ (150, $P321$)	$\langle 2+(1,0,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H312$ (150, $P321$)	$\langle (2;\ 4)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H312$ (150, $P321$)	$\langle 2+(3,4,0);\ 4+(3,3,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,7/3,0$
$H312$ (150, $P321$)	$\langle (2;\ 4)+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H312$ (150, $P321$)	$\langle 2+(2,0,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
$H312$ (150, $P321$)	$\langle 2+(3,-1,0);\ 4+(3,3,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$7/3,2/3,0$
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{a}+2\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R32$ (155)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	
$R32$ (155)	$\langle 2;\ 4+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,1$
$R32$ (155)	$\langle 2;\ 4+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,2$
$R32$ (155)	$\langle 2+(1,0,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$2/3,1/3,0$
$R32$ (155)	$\langle 2+(1,0,0);\ 4+(1,1,2)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$2/3,1/3,1$
$R32$ (155)	$\langle 2+(1,0,0);\ 4+(1,1,4)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$2/3,1/3,2$
$R32$ (155)	$\langle (2;\ 4)+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$1/3,2/3,0$
$R32$ (155)	$\langle 2+(1,1,0);\ 4+(1,1,2)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$1/3,2/3,1$
$R32$ (155)	$\langle 2+(1,1,0);\ 4+(1,1,4)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$1/3,2/3,2$
[3] $\mathbf{a}'=2\mathbf{a}+\mathbf{b},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R32$ (155)	$\langle 2;\ 4\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	
$R32$ (155)	$\langle 2;\ 4+(0,0,2)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,1$
$R32$ (155)	$\langle 2;\ 4+(0,0,4)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,2$
$R32$ (155)	$\langle 2+(1,0,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$2/3,1/3,0$
$R32$ (155)	$\langle 2+(1,0,0);\ 4+(1,1,2)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$2/3,1/3,1$
$R32$ (155)	$\langle 2+(1,0,0);\ 4+(1,1,4)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$2/3,1/3,2$
$R32$ (155)	$\langle (2;\ 4)+(1,1,0)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$1/3,2/3,0$
$R32$ (155)	$\langle 2+(1,1,0);\ 4+(1,1,2)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$1/3,2/3,1$
$R32$ (155)	$\langle 2+(1,1,0);\ 4+(1,1,4)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$1/3,2/3,2$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P312$ (149)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P312$ (149)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P312$ (149)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P312$ (149)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

• **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$P312$ (149)	$\langle 2;\ 4 + (0,0,2u)\rangle$ $p > 2;\ 0 \leq u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P312$ (149)	$\langle 2 + (u+v, -u+2v, 0);\ 4 + (u+v, u+v, 0)\rangle$ $p > 1;\ p \neq 3;\ 0 \leq u < p;\ 0 \leq v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}1m$ (162); [2] $P\bar{3}1c$ (163); [2] $P622$ (177); [2] $P6_322$ (182); [2] $P\bar{6}m2$ (187); [2] $P\bar{6}c2$ (188)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations**

[3] $H312$ (150, $P321$)

• **Decreased unit cell** none

$P321$ No. 150 $P321$ D_3^2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
6 g 1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$
	(4) $y,x,\bar{z}$ (5) $x-y,\bar{y},\bar{z}$ (6) $\bar{x},\bar{x}+y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P311$ (143, $P3$)	1; 2; 3		
[3] $P121$ (5, $C121$)	1; 4	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P121$ (5, $C121$)	1; 5	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
[3] $P121$ (5, $C121$)	1; 6	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P321$ (150)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P321$ (150)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P3_221$ (154)	$\langle 4;\ 2+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P3_221$ (154)	$\langle (2;\ 4)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P3_221$ (154)	$\langle 2+(0,0,2);\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
$P3_121$ (152)	$\langle 4;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P3_121$ (152)	$\langle 2+(0,0,1);\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P3_121$ (152)	$\langle 2+(0,0,1);\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
$P321$ (150)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P321$ (150)	$\langle 2;\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P321$ (150)	$\langle 2;\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H321$ (149, $P312$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P321$ (150)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P321$ (150)	$\langle (2;\ 4)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P321$ (150)	$\langle 2+(1,2,0);\ 4+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P321$ (150)	$\langle 4;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P321$ (150)	$\langle 2;\ 4+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P321$ (150)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}m1$ (164); [2] $P\bar{3}c1$ (165); [2] $P622$ (177); [2] $P6_322$ (182); [2] $P\bar{6}2m$ (189); [2] $P\bar{6}2c$ (190)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $H321$ (149, $P312$); [3] $R_{\mathrm{obv}}32$ (155, $R32$); [3] $R_{\mathrm{rev}}32$ (155, $R32$)

- **Decreased unit cell** none

D_3^3 $P3_112$ No. 151 $P3_112$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$
			(4) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(5) $\bar{x}+y,y,\bar{z}+\frac{1}{3}$	(6) $x,x-y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P3_111$ (144, $P3_1$)	1; 2; 3		
[3] $P112$ (5, $C121$)	1; 6	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,0,1/3$
[3] $P112$ (5, $C121$)	1; 5	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,2/3$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3_212$ (153)	$\langle 4;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P3_212$ (153)	$\langle (2;\ 4)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3_112$ (152, $P3_121$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3_112$ (152, $P3_121$)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H3_112$ (152, $P3_121$)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,-2/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(2,2,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(3,4,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H3_112$ (152, $P3_121$)	$\langle 4;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,-1/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(2,3,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H3_112$ (152, $P3_121$)	$\langle 2+(3,2,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3_112$ (151)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3_112$ (151)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3_112$ (151)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3_112$ (151)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P3_212$ (153)	$\langle 2+(0,0,\frac{2p}{3}-\frac{1}{3});\ 4+(0,0,\frac{p}{3}-\frac{2}{3}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 2 \pmod 3$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P3_112$ (151)	$\langle 2+(0,0,\frac{p}{3}-\frac{1}{3});\ 4+(0,0,\frac{2p}{3}-\frac{2}{3}+2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 3$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3_112$ (151)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_122$ (178); [2] $P6_422$ (181)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H3_112$ (152, $P3_121$)

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P312$ (149)

$P3_121$ No. 152 $P3_121$ D_3^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}+\frac{2}{3}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$

I Maximal *translationengleiche* subgroups

[2] $P3_111$ (144, $P3_1$)	1; 2; 3		
[3] $P121$ (5, $C121$)	1; 4	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P121$ (5, $C121$)	1; 5	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	$0,0,1/3$
[3] $P121$ (5, $C121$)	1; 6	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	$0,0,2/3$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3_221$ (154)	$\langle 4;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P3_221$ (154)	$\langle (2;\ 4)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3_121$ (151, $P3_112$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,1/3$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3_121$ (152)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3_121$ (152)	$\langle (2;\ 4)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3_121$ (152)	$\langle 2+(1,2,0);\ 4+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3_121$ (152)	$\langle 4;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P3_221$ (154)	$\langle 2+(0,0,\frac{2p}{3}-\frac{1}{3});\ 4+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 2$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P3_121$ (152)	$\langle 2+(0,0,\frac{p}{3}-\frac{1}{3});\ 4+(0,0,2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3_121$ (152)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_122$ (178); [2] $P6_422$ (181)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H3_121$ (151, $P3_112$); [3] $R_{\mathrm{obv}}32$ (155, $R32$); [3] $R_{\mathrm{rev}}32$ (155, $R32$)

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P321$ (150)

D_3^5 $P3_212$ No. 153 $P3_212$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$
			(4) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(5) $\bar{x}+y,y,\bar{z}+\frac{2}{3}$	(6) $x,x-y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P3_211$ (145, $P3_2$)	1; 2; 3		
[3] $P112$ (5, $C121$)	1; 6	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P112$ (5, $C121$)	1; 5	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,1/3$
[3] $P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,0,2/3$

II Maximal *klassengleiche* subgroups

• **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3_112$ (151)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P3_112$ (151)	$\langle 2;\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3_212$ (154, $P3_221$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3_212$ (154, $P3_221$)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H3_212$ (154, $P3_221$)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H3_212$ (154, $P3_221$)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,-2/3,0$
$H3_212$ (154, $P3_221$)	$\langle 2+(2,2,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3_212$ (154, $P3_221$)	$\langle 2+(3,4,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H3_212$ (154, $P3_221$)	$\langle 4;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,-1/3,0$
$H3_212$ (154, $P3_221$)	$\langle 2+(2,3,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H3_212$ (154, $P3_221$)	$\langle 2+(3,2,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3_212$ (153)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3_212$ (153)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3_212$ (153)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3_212$ (153)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

• **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P3_212$ (153)	$\langle 2+(0,0,\frac{2p}{3}-\frac{2}{3});\ 4+(0,0,\frac{p}{3}-\frac{1}{3}+2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P3_112$ (151)	$\langle 2+(0,0,\frac{p}{3}-\frac{2}{3});\ 4+(0,0,\frac{2p}{3}-\frac{1}{3}+2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 2$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3_212$ (153)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_522$ (179); [2] $P6_222$ (180)

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations**

[3] $H3_212$ (154, $P3_221$)

• **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P312$ (149)

$P3_221$ No. 154 $P3_221$ D_3^6

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
6	c	1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{2}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$
			(4) $y,x,\bar{z}$ (5) $x-y,\bar{y},\bar{z}+\frac{1}{3}$ (6) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$

I Maximal *translationengleiche* subgroups

[2] $P3_211$ (145, $P3_2$)	1; 2; 3		
[3] $P121$ (5, $C121$)	1; 4	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P121$ (5, $C121$)	1; 6	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	$0,0,1/3$
[3] $P121$ (5, $C121$)	1; 5	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	$0,0,2/3$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3_121$ (152)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P3_121$ (152)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3_221$ (153, $P3_212$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,1/6$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3_221$ (154)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3_221$ (154)	$\langle (2;\ 4)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3_221$ (154)	$\langle 2+(1,2,0);\ 4+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3_221$ (154)	$\langle 4;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P3_221$ (154)	$\langle 2+(0,0,\frac{2p}{3}-\frac{2}{3});\ 4+(0,0,2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 3$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P3_121$ (152)	$\langle 2+(0,0,\frac{p}{3}-\frac{2}{3});\ 4+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 2 \pmod 3$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3_221$ (154)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_522$ (179); [2] $P6_222$ (180)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H3_221$ (153, $P3_212$); [3] $R_{\text{obv}}32$ (155, $R32$); [3] $R_{\text{rev}}32$ (155, $R32$)

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P321$ (150)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 155, pp. 295–297.

D_3^7 $R32$ No. 155 $R32$

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
			$(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
18	f	1	(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$
			(4) $y,x,\bar{z}$ (5) $x-y,\bar{y},\bar{z}$ (6) $\bar{x},\bar{x}+y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $R31$ (146, $R3$)	(1; 2; 3)+		
[3] $R12$ (5, $C121$)	(1; 4)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}),-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $R12$ (5, $C121$)	(1; 5)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}),\mathbf{a},\mathbf{c}$	
[3] $R12$ (5, $C121$)	(1; 6)+	$1/3(2\mathbf{a}+\mathbf{b}-2\mathbf{c}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[3] $P3_221$ (154)	1; 4; (2; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; (3; 5) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		$2/3,2/3,0$
[3] $P3_221$ (154)	1; 5; (2; 4) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; (3; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		$1/3,0,1/3$
[3] $P3_221$ (154)	1; 6; (2; 5) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$; (3; 4) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		$0,1/3,2/3$
[3] $P3_121$ (152)	1; 4; (2; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (3; 5) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		$1/3,1/3,0$
[3] $P3_121$ (152)	1; 5; (2; 4) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (3; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		$2/3,0,2/3$
[3] $P3_121$ (152)	1; 6; (2; 5) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (3; 4) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		$0,2/3,1/3$
[3] $P321$ (150)	1; 2; 3; 4; 5; 6		
[3] $P321$ (150)	1; 2; 3; (4; 5; 6) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		$2/3,1/3,1/3$
[3] $P321$ (150)	1; 2; 3; (4; 5; 6) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		$1/3,2/3,2/3$

- **Enlarged unit cell**

[2] $\mathbf{a}'=-\mathbf{b}$, $\mathbf{b}'=\mathbf{a}+\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$R32$ (155)	$\langle 2;\ 4\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$R32$ (155)	$\langle 2;\ 4+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$			
$R32$ (155)	$\langle 2;\ 4\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$R32$ (155)	$\langle (2;\ 4)+(1,-1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$R32$ (155)	$\langle 2+(1,2,0);\ 4+(-1,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,1,0$
$R32$ (155)	$\langle 4;\ 2+(2,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$R32$ (155)	$\langle 2;\ 4+(0,0,2u)\rangle$ $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 2$ (mod 3)	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	$0,0,u$
$R32$ (155)	$\langle 2;\ 4+(0,0,2u)\rangle$ $p>6$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$R32$ (155)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0)\rangle$ $p>1$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2$ (mod 3)	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$
$R32$ (155)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0)\rangle$ $p>6$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1$ (mod 3)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $P432$ (207); [4] $P4_232$ (208); [4] $F432$ (209); [4] $F4_132$ (210); [4] $I432$ (211); [4] $P4_332$ (212); [4] $P4_132$ (213); [4] $I4_132$ (214)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$, $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$, $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P312$ (149)

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	f	1	(1) x,y,z	(2) z,x,y	(3) y,z,x
			(4) $\bar{z},\bar{y},\bar{x}$	(5) $\bar{y},\bar{x},\bar{z}$	(6) $\bar{x},\bar{z},\bar{y}$

I Maximal *translationengleiche* subgroups

[2] $R31$ (146, $R3$)	1; 2; 3		
[3] $R12$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{c}, -\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	
[3] $R12$ (5, $C121$)	1; 5	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	
[3] $R12$ (5, $C121$)	1; 6	$-\mathbf{b}-\mathbf{c}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell**

[2] $\mathbf{a}'=\mathbf{a}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b},\ \mathbf{c}'=\mathbf{b}+\mathbf{c}$

$R32$ (155)	$\langle 2;\ 4\rangle$	$\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}$	
$R32$ (155)	$\langle 2;\ 4+(1,1,1)\rangle$	$\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}$	$1/2, 1/2, 1/2$

[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{b}-\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$

$P3_221$ (154)	$\langle 4;\ 2+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$2/3, 0, -2/3$
$P3_221$ (154)	$\langle (2;\ 4)+(1,0,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$2/3, 0, 1/3$
$P3_221$ (154)	$\langle 2+(1,1,0);\ 4+(1,2,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$2/3, 1, 1/3$
$P3_121$ (152)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/3, 0, -1/3$
$P3_121$ (152)	$\langle 2+(1,-1,1);\ 4+(2,0,2)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$4/3, 0, 2/3$
$P3_121$ (152)	$\langle 2+(1,1,-1);\ 4+(0,2,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/3, 1, -1/3$
$P321$ (150)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	
$P321$ (150)	$\langle 2+(1,-1,0);\ 4+(1,0,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1, 0, 0$
$P321$ (150)	$\langle 2+(1,0,-1);\ 4+(1,2,1)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1, 1, 0$

[4] $\mathbf{a}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b}-\mathbf{c},\ \mathbf{c}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}$

$R32$ (155)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	
$R32$ (155)	$\langle (2;\ 4)+(1,-2,1)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1, -1, 0$
$R32$ (155)	$\langle 2+(1,1,-2);\ 4+(-1,2,-1)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0, 1, -1$
$R32$ (155)	$\langle 4;\ 2+(2,-1,-1)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1, 0, -1$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p-2)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(p-2)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-2)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R32$ (155) $\langle 2;\ 4+(2u,2u,2u)\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
$p>4;\ 0\le u<p$ u,u,u
p conjugate subgroups for prime $p\equiv 2$ (mod 3)

[p] $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}+(p-1)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p+2)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p-1)\mathbf{b}+(p+2)\mathbf{c}\big)$

$R32$ (155) $\langle 2;\ 4+(2u,2u,2u)\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations
$p>6;\ 0\le u<p$ u,u,u
p conjugate subgroups for prime $p\equiv 1$ (mod 3)

[p^2] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R32$ (155) $\langle 2+(u+v,-2u+v,u-2v);$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
$4+(u-v,-2u+2v,u-v)\rangle$ $u,-u+v,-v$
$p>1;\ 0\le u<p;\ 0\le v<p$
p^2 conjugate subgroups for prime $p\equiv 2$ (mod 3)

[p^2] $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}+(1-p)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((1-p)\mathbf{a}+(2p+1)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-p)\mathbf{a}+(1-p)\mathbf{b}+(2p+1)\mathbf{c}\big)$

$R32$ (155) $\langle 2+(u+v,-2u+v,u-2v);$ $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}\ldots$, see lattice relations
$4+(u-v,-2u+2v,u-v)\rangle$ $u,-u+v,-v$
$p>6;\ 0\le u<p;\ 0\le v<p$
p^2 conjugate subgroups for prime $p\equiv 1$ (mod 3)

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}m$ (166); [2] $R\bar{3}c$ (167); [4] $P432$ (207); [4] $P4_232$ (208); [4] $F432$ (209); [4] $F4_132$ (210); [4] $I432$ (211); [4] $P4_332$ (212); [4] $P4_132$ (213); [4] $I4_132$ (214)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c}),\ \mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c}),\ \mathbf{c}' = \frac{1}{3}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ $P312$ (149)

$P3m1$ No. 156 $P3m1$ C_{3v}^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	e	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$

I Maximal *translationengleiche* subgroups

[2] $P311$ (143, $P3$)	1; 2; 3		
[3] $P1m1$ (8, $C1m1$)	1; 4	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P1m1$ (8, $C1m1$)	1; 5	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
[3] $P1m1$ (8, $C1m1$)	1; 6	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P3c1$ (158)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P3m1$ (156)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
$P3m1$ (156)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3m1$ (157, $P31m$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3m1$ (157, $P31m$)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H3m1$ (157, $P31m$)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H3m1$ (157, $P31m$)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,-2/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(2,2,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(3,4,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H3m1$ (157, $P31m$)	$\langle 4;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,-1/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(2,3,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H3m1$ (157, $P31m$)	$\langle 2+(3,2,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3m1$ (156)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3m1$ (156)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3m1$ (156)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3m1$ (156)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P3m1$ (156)	$\langle 2;\ 4\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3m1$ (156)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}m1$ (164); [2] $P6mm$ (183); [2] $P6_3mc$ (186); [2] $P\bar{6}m2$ (187)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H3m1$ (157, $P31m$); [3] $R_{\mathrm{obv}}3m$ (160, $R3m$); [3] $R_{\mathrm{rev}}3m$ (160, $R3m$)

- **Decreased unit cell** none

C_{3v}^2 $P31m$ No. 157 $P31m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) y,x,z	(5) $x-y,\bar{y},z$	(6) $\bar{x},\bar{x}+y,z$

I Maximal *translationengleiche* subgroups

[2] $P311$ (143, $P3$)	1; 2; 3		
{ [3] $P11m$ (8, $C1m1$)	1; 4	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	
{ [3] $P11m$ (8, $C1m1$)	1; 5	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ [3] $P11m$ (8, $C1m1$)	1; 6	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P31c$ (159)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P31m$ (157)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
$P31m$ (157)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H31m$ (156, $P3m1$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{a}+2\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R3m$ (160)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=2\mathbf{a}+\mathbf{b},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R3m$ (160)	$\langle 2;\ 4\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P31m$ (157)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P31m$ (157)	$\langle (2;\ 4)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P31m$ (157)	$\langle 2+(1,2,0);\ 4+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P31m$ (157)	$\langle 4;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P31m$ (157)	$\langle 2;\ 4\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P31m$ (157)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}1m$ (162); [2] $P6mm$ (183); [2] $P6_3cm$ (185); [2] $P\bar{6}2m$ (189)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H31m$ (156, $P3m1$)

- **Decreased unit cell** none

$P3c1$ No. 158 $P3c1$ C_{3v}^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P311$ (143, $P3$)	1; 2; 3		
[3] $P1c1$ (9, $C1c1$)	1; 4	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P1c1$ (9, $C1c1$)	1; 5	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
[3] $P1c1$ (9, $C1c1$)	1; 6	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P3c1$ (158)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H3c1$ (159, $P31c$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H3c1$ (159, $P31c$)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H3c1$ (159, $P31c$)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H3c1$ (159, $P31c$)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,-2/3,0$
$H3c1$ (159, $P31c$)	$\langle 2+(2,2,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H3c1$ (159, $P31c$)	$\langle 2+(3,4,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H3c1$ (159, $P31c$)	$\langle 4;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,-1/3,0$
$H3c1$ (159, $P31c$)	$\langle 2+(2,3,0);\ 4+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H3c1$ (159, $P31c$)	$\langle 2+(3,2,0);\ 4+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P3c1$ (158)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P3c1$ (158)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P3c1$ (158)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P3c1$ (158)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P3c1$ (158)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P3c1$ (158)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}c1$ (165); [2] $P6cc$ (184); [2] $P6_3cm$ (185); [2] $P\bar{6}c2$ (188)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H3c1$ (159, $P31c$); [3] $R_{\text{obv}}3c$ (161, $R3c$); [3] $R_{\text{rev}}3c$ (161, $R3c$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P3m1$ (156)

C_{3v}^4 $P31c$ No. 159 $P31c$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $y,x,z+\frac{1}{2}$	(5) $x-y,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P311$ (143, $P3$)	1; 2; 3		
[3] $P11c$ (9, $C1c1$)	1; 4	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P11c$ (9, $C1c1$)	1; 5	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
[3] $P11c$ (9, $C1c1$)	1; 6	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P31c$ (159)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H31c$ (158, $P3c1$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{a}+2\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R3c$ (161)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=2\mathbf{a}+\mathbf{b},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
$R3c$ (161)	$\langle 2;\ 4+(0,0,1)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P31c$ (159)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P31c$ (159)	$\langle(2;\ 4)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P31c$ (159)	$\langle 2+(1,2,0);\ 4+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P31c$ (159)	$\langle 4;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P31c$ (159)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P31c$ (159)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P\bar{3}1c$ (163); [2] $P6cc$ (184); [2] $P6_3mc$ (186); [2] $P\bar{6}2c$ (190)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H31c$ (158, $P3c1$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P31m$ (157)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 160, pp. 302–303.

$R3m$ No. 160 $R3m$ C_{3v}^5

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
18	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$

I Maximal *translationengleiche* subgroups

[2] $R31$ (146, $R3$)	(1; 2; 3)+		
[3] $R1m$ (8, $C1m1$)	(1; 4)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}),-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $R1m$ (8, $C1m1$)	(1; 5)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}),\mathbf{a},\mathbf{c}$	
[3] $R1m$ (8, $C1m1$)	(1; 6)+	$1/3(2\mathbf{a}+\mathbf{b}-2\mathbf{c}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[3] $P3m1$ (156)	1; 2; 3; 4; 5; 6		

- **Enlarged unit cell**

[2] $\mathbf{a}'=-\mathbf{b}$, $\mathbf{b}'=\mathbf{a}+\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$R3m$ (160)	$\langle 2;\ 4\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
[2] $\mathbf{a}'=\mathbf{a}+\mathbf{b}$, $\mathbf{b}'=-\mathbf{a}$, $\mathbf{c}'=2\mathbf{c}$			
$R3c$ (161)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a}+\mathbf{b},-\mathbf{a},2\mathbf{c}$	
[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$			
$R3m$ (160)	$\langle 2;\ 4\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$R3m$ (160)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$R3m$ (160)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,1,0$
$R3m$ (160)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$R3m$ (160)	$\langle 2;\ 4\rangle$ $p>1$; $p\equiv 2$ (mod 3) no conjugate subgroups	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	
$R3m$ (160)	$\langle 2;\ 4\rangle$ $p>6$; $p\equiv 1$ (mod 3) no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=-p\mathbf{b}$, $\mathbf{b}'=p\mathbf{a}+p\mathbf{b}$			
$R3m$ (160)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2$ (mod 3)	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p^2]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$R3m$ (160)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>6$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1$ (mod 3)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}m$ (166); [4] $P\bar{4}3m$ (215); [4] $F\bar{4}3m$ (216); [4] $I\bar{4}3m$ (217)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$, $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$, $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P31m$ (157)

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates
6	c	1	(1) x,y,z (2) z,x,y (3) y,z,x (4) z,y,x (5) y,x,z (6) x,z,y

I Maximal *translationengleiche* subgroups

[2] $R31$ (146, $R3$)	1; 2; 3	
{ [3] $R1m$ (8, $C1m1$)	1; 4	$-\mathbf{a}-\mathbf{c},-\mathbf{a}+\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$
{ [3] $R1m$ (8, $C1m1$)	1; 5	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b}+\mathbf{c}$
{ [3] $R1m$ (8, $C1m1$)	1; 6	$-\mathbf{b}-\mathbf{c},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell**

[2] $\mathbf{a}'=\mathbf{a}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b},\ \mathbf{c}'=\mathbf{b}+\mathbf{c}$

$R3m$ (160)	$\langle 2;\,4\rangle$	$\mathbf{a}+\mathbf{c},\mathbf{a}+\mathbf{b},\mathbf{b}+\mathbf{c}$	

[2] $\mathbf{a}'=\mathbf{a}+\mathbf{b},\ \mathbf{b}'=\mathbf{b}+\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{c}$

$R3c$ (161)	$\langle 2;\,4+(1,1,1)\rangle$	$\mathbf{a}+\mathbf{b},\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{c}$	

[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{b}-\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$

$P3m1$ (156)	$\langle 2;\,4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	

[4] $\mathbf{a}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b}-\mathbf{c},\ \mathbf{c}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}$

{ $R3m$ (160)	$\langle 2;\,4\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ $R3m$ (160)	$\langle 2+(1,-2,1);\,4+(1,0,-1)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,-1,0$
{ $R3m$ (160)	$\langle 2+(1,1,-2);\,4+(1,0,-1)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0,1,-1$
{ $R3m$ (160)	$\langle 2+(2,-1,-1);\,4+(2,0,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,-1$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p-2)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(p-2)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-2)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R3m$ (160)	$\langle 2;\,4\rangle$ $p>1;\ p\equiv 2 \pmod 3$ no conjugate subgroups	$\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations	

$[p]$ $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}+(p-1)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p+2)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p-1)\mathbf{b}+(p+2)\mathbf{c}\big)$

$R3m$ (160)	$\langle 2;\,4\rangle$ $p>6;\ p\equiv 1 \pmod 3$ no conjugate subgroups	$\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations	

$[p^2]$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R3m$ (160)	$\langle 2+(u+v,-2u+v,u-2v);\,4+(u+v,0,-u-v)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations	$u,-u+v,-v$

$[p^2]$ $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}+(1-p)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((1-p)\mathbf{a}+(2p+1)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-p)\mathbf{a}+(1-p)\mathbf{b}+(2p+1)\mathbf{c}\big)$

$R3m$ (160)	$\langle 2+(u+v,-2u+v,u-2v);\,4+(u+v,0,-u-v)\rangle$ $p>6;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1 \pmod 3$	$\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}\ldots$, see lattice relations	$u,-u+v,-v$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}m$ (166); [4] $P\bar{4}3m$ (215); [4] $F\bar{4}3m$ (216); [4] $I\bar{4}3m$ (217)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\ \mathbf{b}'=\frac{1}{3}(\mathbf{a}+2\mathbf{b}-\mathbf{c}),\ \mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ $P31m$ (157)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 161, pp. 304–305.

$R3c$ No. 161 $R3c$ C_{3v}^6

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$		
18 *b* 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
	(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $R31$ (146, $R3$)	(1; 2; 3)+		
[3] $R1c$ (9, $C1c1$)	(1; 4)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}),-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $R1c$ (9, $C1c1$)	(1; 5)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}),\mathbf{a},\mathbf{c}$	
[3] $R1c$ (9, $C1c1$)	(1; 6)+	$1/3(2\mathbf{a}+\mathbf{b}-2\mathbf{c}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[3] $P3c1$ (158) 1; 2; 3; 4; 5; 6

- **Enlarged unit cell**

[4] $\mathbf{a}'=-2\mathbf{b},\ \mathbf{b}'=2\mathbf{a}+2\mathbf{b}$

$R3c$ (161)	$\langle 2;\ 4\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$R3c$ (161)	$\langle 2+(1,-1,0);\ 4+(1,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$R3c$ (161)	$\langle 2+(1,2,0);\ 4+(1,1,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,1,0$
$R3c$ (161)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$R3c$ (161)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>4;\ p\equiv 5 \pmod 6$ no conjugate subgroups	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	
$R3c$ (161)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>6;\ p\equiv 1 \pmod 6$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

$[p^2]$ $\mathbf{a}'=-p\mathbf{b},\ \mathbf{b}'=p\mathbf{a}+p\mathbf{b}$

$R3c$ (161)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$

$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$

$R3c$ (161)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0)\rangle$ $p>6;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}c$ (167); [4] $P\bar{4}3n$ (218); [4] $F\bar{4}3c$ (219); [4] $I\bar{4}3d$ (220)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b}),\ \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b}),\ \mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P31c$ (159); [2] $\mathbf{a}'=-\mathbf{a},\ \mathbf{b}'=-\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $R3m$ (160)

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	b	1	(1) x,y,z	(2) z,x,y	(3) y,z,x
			(4) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(5) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(6) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $R31$ (146, $R3$)	1; 2; 3		
[3] $R1c$ (9, $C1c1$)	1; 4	$-\mathbf{a}-\mathbf{c},-\mathbf{a}+\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[3] $R1c$ (9, $C1c1$)	1; 5	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[3] $R1c$ (9, $C1c1$)	1; 6	$-\mathbf{b}-\mathbf{c},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{b}-\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$

$P3c1$ (158)	$\langle 2;\,4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	

[4] $\mathbf{a}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b}-\mathbf{c},\ \mathbf{c}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}$

$R3c$ (161)	$\langle 2;\,4\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	
$R3c$ (161)	$\langle 2+(1,-2,1);\,4+(1,0,-1)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,-1,0$
$R3c$ (161)	$\langle 2+(1,1,-2);\,4+(1,0,-1)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0,1,-1$
$R3c$ (161)	$\langle 2+(2,-1,-1);\,4+(2,0,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,-1$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p-2)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(p-2)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-2)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R3c$ (161) $\langle 2;\,4+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2})\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
$p>4;\ p\equiv 5 \pmod 6$
no conjugate subgroups

[p] $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}+(p-1)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p+2)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p-1)\mathbf{b}+(p+2)\mathbf{c}\big)$

$R3c$ (161) $\langle 2;\,4+(\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2})\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations
$p>6;\ p\equiv 1 \pmod 6$
no conjugate subgroups

[p^2] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R3c$ (161) $\langle 2+(u+v,-2u+v,u-2v);\,4+(u+v,0,-u-v)\rangle$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
$p>1;\ 0\le u<p;\ 0\le v<p$ $u,-u+v,-v$
p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$

[p^2] $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}+(1-p)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((1-p)\mathbf{a}+(2p+1)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-p)\mathbf{a}+(1-p)\mathbf{b}+(2p+1)\mathbf{c}\big)$

$R3c$ (161) $\langle 2+(u+v,-2u+v,u-2v);\,4+(u+v,0,-u-v)\rangle$ $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}\ldots$, see lattice relations
$p>6;\ 0\le u<p;\ 0\le v<p$ $u,-u+v,-v$
p^2 conjugate subgroups for prime $p\equiv 1 \pmod 3$

I Minimal *translationengleiche* supergroups

[2] $R\bar{3}c$ (167); [4] $P\bar{4}3n$ (218); [4] $F\bar{4}3c$ (219); [4] $I\bar{4}3d$ (220)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})),\ \mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\ \mathbf{c}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ $P31c$ (159);
[2] $\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\ \mathbf{b}'=\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\ \mathbf{c}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$ $R3m$ (160)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 162, pp. 306–307.

$P\bar{3}1m$ No. 162 $P\bar{3}12/m$ D_{3d}^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},\bar{z}$	(5) $\bar{x}+y,y,\bar{z}$	(6) $x,x-y,\bar{z}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$

I Maximal *translationengleiche* subgroups

[2] $P31m$ (157)	1; 2; 3; 10; 11; 12		
[2] $P312$ (149)	1; 2; 3; 4; 5; 6		
[2] $P\bar{3}11$ (147, $P\bar{3}$)	1; 2; 3; 7; 8; 9		
{ [3] $P112/m$ (12, $C12/m1$)	1; 4; 7; 10		$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$
{ [3] $P112/m$ (12, $C12/m1$)	1; 5; 7; 11		$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$
{ [3] $P112/m$ (12, $C12/m1$)	1; 6; 7; 12		$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{3}1c$ (163)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{3}1c$ (163)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{3}1m$ (162)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{3}1m$ (162)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{3}1m$ (162)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{3}1m$ (162)	$\langle 2;\ (4;\ 7)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{3}1m$ (162)	$\langle 2;\ (4;\ 7)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H\bar{3}1m$ (164, $P\bar{3}m1$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H\bar{3}1m$ (164, $P\bar{3}m1$)	$\langle 2+(1,-1,0);\ 4+(1,1,0);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H\bar{3}1m$ (164, $P\bar{3}m1$)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{a}+2\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
{ $R\bar{3}m$ (166)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	
{ $R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=2\mathbf{a}+\mathbf{b},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
{ $R\bar{3}m$ (166)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	
{ $R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(0,0,2)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(0,0,4)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,2$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P\bar{3}1m$ (162)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P\bar{3}1m$ (162)	$\langle 2+(1,-1,0);\ 4+(1,1,0);\ 7+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P\bar{3}1m$ (162)	$\langle 2+(1,2,0);\ 4+(1,1,0);\ 7+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P\bar{3}1m$ (162)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{3}1m$ (162)	$\langle 2;\ (4;\ 7)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{3}1m$ (162)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0);$ $7+(2u,2v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191); [2] $P6_3/mcm$ (193)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{3}1m$ (164, $P\bar{3}m1$)

- **Decreased unit cell** none

$P\bar{3}1c$ No. 163 $P\bar{3}12/c$ D_{3d}^{2}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	*i*	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(5) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(6) $x,x-y,\bar{z}+\frac{1}{2}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P31c$ (159)	1; 2; 3; 10; 11; 12		
[2] $P312$ (149)	1; 2; 3; 4; 5; 6		$0,0,1/4$
[2] $P\bar{3}11$ (147, $P\bar{3}$)	1; 2; 3; 7; 8; 9		
{ [3] $P112/c$ (15, $C12/c1$)	1; 4; 7; 10	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	
{ [3] $P112/c$ (15, $C12/c1$)	1; 5; 7; 11	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ [3] $P112/c$ (15, $C12/c1$)	1; 6; 7; 12	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{3}1c$ (163)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{3}1c$ (163)	$\langle 2;\ 4+(0,0,3);\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{3}1c$ (163)	$\langle 2;\ 4+(0,0,5);\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H\bar{3}1c$ (165, $P\bar{3}c1$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H\bar{3}1c$ (165, $P\bar{3}c1$)	$\langle 2+(1,-1,0);\ 4+(1,1,0);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H\bar{3}1c$ (165, $P\bar{3}c1$)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{a}+2\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
{ $R\bar{3}c$ (167)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	
{ $R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,3);\ 7+(0,0,2)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,5);\ 7+(0,0,4)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=2\mathbf{a}+\mathbf{b},\ \mathbf{b}'=-\mathbf{a}+\mathbf{b},\ \mathbf{c}'=3\mathbf{c}$			
{ $R\bar{3}c$ (167)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	
{ $R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,3);\ 7+(0,0,2)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,5);\ 7+(0,0,4)\rangle$	$2\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b},3\mathbf{c}$	$0,0,2$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P\bar{3}1c$ (163)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P\bar{3}1c$ (163)	$\langle 2+(1,-1,0);\ 4+(1,1,0);\ 7+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P\bar{3}1c$ (163)	$\langle 2+(1,2,0);\ 4+(1,1,0);\ 7+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P\bar{3}1c$ (163)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{3}1c$ (163)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{3}1c$ (163)	$\langle 2+(u+v,-u+2v,0);\ 4+(u+v,u+v,0);$ $7+(2u,2v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mcc$ (192); [2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{3}1c$ (165, $P\bar{3}c1$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{3}1m$ (162)

D_{3d}^3 $P\bar{3}2/m1$ No. 164 $P\bar{3}m1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	j	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$

I Maximal *translationengleiche* subgroups

[2] $P3m1$ (156)	1; 2; 3; 10; 11; 12	
[2] $P321$ (150)	1; 2; 3; 4; 5; 6	
[2] $P\bar{3}11$ (147, $P\bar{3}$)	1; 2; 3; 7; 8; 9	
{ [3] $P12/m1$ (12, $C12/m1$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$
{ [3] $P12/m1$ (12, $C12/m1$)	1; 5; 7; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$
{ [3] $P12/m1$ (12, $C12/m1$)	1; 6; 7; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{3}c1$ (165)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{3}c1$ (165)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{3}m1$ (164)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{3}m1$ (164)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=3\mathbf{b}$			
{ $H\bar{3}m1$ (162, $P\bar{3}1m$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H\bar{3}m1$ (162, $P\bar{3}1m$)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H\bar{3}m1$ (162, $P\bar{3}1m$)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$			
{ $P\bar{3}m1$ (164)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P\bar{3}m1$ (164)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P\bar{3}m1$ (164)	$\langle 2+(1,2,0);\ 4+(-1,1,0);\ 7+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P\bar{3}m1$ (164)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{3}m1$ (164)	$\langle 2;\ (4;\ 7)+(0,0,2u)\rangle$ $p>2$; $0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$P\bar{3}m1$ (164)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);$ $7+(2u,2v,0)\rangle$ $p>1$; $p\neq 3$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{3}m1$ (162, $P\bar{3}1m$); [3] $R_{\mathrm{obv}}\bar{3}m$ (166, $R\bar{3}m$); [3] $R_{\mathrm{rev}}\bar{3}m$ (166, $R\bar{3}m$)

- **Decreased unit cell** none

$P\bar{3}c1$ No. 165 $P\bar{3}2/c1$ D_{3d}^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P3c1$ (158)	1; 2; 3; 10; 11; 12		
[2] $P321$ (150)	1; 2; 3; 4; 5; 6		$0,0,1/4$
[2] $P\bar{3}11$ (147, $P\bar{3}$)	1; 2; 3; 7; 8; 9		
[3] $P12/c1$ (15, $C12/c1$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P12/c1$ (15, $C12/c1$)	1; 5; 7; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
[3] $P12/c1$ (15, $C12/c1$)	1; 6; 7; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P\bar{3}c1$ (165)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{3}c1$ (165)	$\langle 2;\ 4+(0,0,3);\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{3}c1$ (165)	$\langle 2;\ 4+(0,0,5);\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H\bar{3}c1$ (163, $P\bar{3}1c$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H\bar{3}c1$ (163, $P\bar{3}1c$)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H\bar{3}c1$ (163, $P\bar{3}1c$)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P\bar{3}c1$ (165)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P\bar{3}c1$ (165)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{3}c1$ (165)	$\langle 2+(1,2,0);\ 4+(-1,1,0);\ 7+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P\bar{3}c1$ (165)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{3}c1$ (165)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{3}c1$ (165)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);$ $7+(2u,2v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mcc$ (192); [2] $P6_3/mcm$ (193)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{3}c1$ (163, $P\bar{3}1c$); [3] $R_{\mathrm{obv}}\bar{3}c$ (167, $R\bar{3}c$); [3] $R_{\mathrm{rev}}\bar{3}c$ (167, $R\bar{3}c$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{3}m1$ (164)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 166, pp. 311–313.

D_{3d}^5 $R\bar{3}2/m$ No. 166 $R\bar{3}m$

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
36	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$

I Maximal *translationengleiche* subgroups

[2] $R3m$ (160)	(1; 2; 3; 10; 11; 12)+	
[2] $R32$ (155)	(1; 2; 3; 4; 5; 6)+	
[2] $R\bar{3}1$ (148, $R\bar{3}$)	(1; 2; 3; 7; 8; 9)+	
{ [3] $R12/m$ (12, $C12/m1$)	(1; 4; 7; 10)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}),-\mathbf{a}-\mathbf{b},\mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	(1; 5; 7; 11)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}),\mathbf{a},\mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	(1; 6; 7; 12)+	$1/3(2\mathbf{a}+\mathbf{b}-2\mathbf{c}),\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		$1/3,2/3,2/3$
{ [3] $P\bar{3}m1$ (164)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		$2/3,1/3,1/3$

- **Enlarged unit cell**

[2] $\mathbf{a}'=-\mathbf{b}$, $\mathbf{b}'=\mathbf{a}+\mathbf{b}$, $\mathbf{c}'=2\mathbf{c}$			
$R\bar{3}m$ (166)	$\langle 2;\ 4;\ 7\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	
$R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[2] $\mathbf{a}'=\mathbf{a}+\mathbf{b}$, $\mathbf{b}'=-\mathbf{a}$, $\mathbf{c}'=2\mathbf{c}$			
$R\bar{3}c$ (167)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a}+\mathbf{b},-\mathbf{a},2\mathbf{c}$	
$R\bar{3}c$ (167)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$-\mathbf{a},-\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$			
{ $R\bar{3}m$ (166)	$\langle 2;\ 4;\ 7\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $R\bar{3}m$ (166)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $R\bar{3}m$ (166)	$\langle 2+(1,2,0);\ 4+(-1,1,0);\ 7+(0,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $R\bar{3}m$ (166)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(0,0,2u)\rangle$ $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 2$ (mod 3)	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	$0,0,u$
$R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(0,0,2u)\rangle$ $p>6$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$			
$R\bar{3}m$ (166)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);$ $7+(2u,2v,0)\rangle$ $p>6$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 1$ (mod 3)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[p^2] $\mathbf{a}'=-p\mathbf{b}$, $\mathbf{b}'=p\mathbf{a}+p\mathbf{b}$			
$R\bar{3}m$ (166)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);$ $7+(2u,2v,0)\rangle$ $p>1$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2$ (mod 3)	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b}),\ \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b}),\ \mathbf{c}' = \frac{1}{3}\mathbf{c}$ $P\bar{3}1m$ (162)

$R\bar{3}m$ RHOMBOHEDRAL AXES No. 166

(*Continued from the facing page*)

I Minimal *translationengleiche* supergroups

[4] $Pm\bar{3}m$ (221); [4] $Pn\bar{3}m$ (224); [4] $Fm\bar{3}m$ (225); [4] $Fd\bar{3}m$ (227); [4] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\ \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\ \mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ $P\bar{3}1m$ (162)

D_{3d}^5 $\quad$ $R\bar{3}2/m$ $\quad$ No. 166 $\quad$ $R\bar{3}m$

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	i	1	(1) x,y,z	(2) z,x,y	(3) y,z,x
			(4) $\bar{z},\bar{y},\bar{x}$	(5) $\bar{y},\bar{x},\bar{z}$	(6) $\bar{x},\bar{z},\bar{y}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$
			(10) z,y,x	(11) y,x,z	(12) x,z,y

I Maximal *translationengleiche* subgroups

[2] $R3m$ (160)	1; 2; 3; 10; 11; 12	
[2] $R32$ (155)	1; 2; 3; 4; 5; 6	
[2] $R\bar{3}1$ (148, $R\bar{3}$)	1; 2; 3; 7; 8; 9	
{ [3] $R12/m$ (12, $C12/m1$)	1; 4; 7; 10	$-\mathbf{a}-\mathbf{c}, -\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	1; 5; 7; 11	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}+\mathbf{c}$
{ [3] $R12/m$ (12, $C12/m1$)	1; 6; 7; 12	$-\mathbf{b}-\mathbf{c}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** $\quad$ none

- **Enlarged unit cell**

[2] $\mathbf{a}'=\mathbf{a}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b},\ \mathbf{c}'=\mathbf{b}+\mathbf{c}$			
$R\bar{3}m$ (166)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}$	
$R\bar{3}m$ (166)	$\langle 2;\ (4;\ 7)+(1,1,1)\rangle$	$\mathbf{a}+\mathbf{c}, \mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}$	$1/2, 1/2, 1/2$
[2] $\mathbf{a}'=\mathbf{a}+\mathbf{b},\ \mathbf{b}'=\mathbf{b}+\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{c}$			
$R\bar{3}c$ (167)	$\langle 2;\ 7;\ 4+(1,1,1)\rangle$	$\mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{c}$	
$R\bar{3}c$ (167)	$\langle 2;\ 4;\ 7+(1,1,1)\rangle$	$\mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{c}$	$1/2, 1/2, 1/2$
[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{b}-\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$			
{ $P\bar{3}m1$ (164)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ $P\bar{3}m1$ (164)	$\langle 2+(1,-1,0);\ 4+(1,0,1);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,0$
{ $P\bar{3}m1$ (164)	$\langle 2+(1,0,-1);\ 4+(1,2,1);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b}-\mathbf{c},\ \mathbf{c}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}$			
{ $R\bar{3}m$ (166)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ $R\bar{3}m$ (166)	$\langle (2;\ 4)+(1,-2,1);\ 7+(2,-2,0)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,-1,0$
{ $R\bar{3}m$ (166)	$\langle 2+(1,1,-2);\ 4+(-1,2,-1);\ 7+(0,2,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$0,1,-1$
{ $R\bar{3}m$ (166)	$\langle 4;\ 2+(2,-1,-1);\ 7+(2,0,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{b}-\mathbf{c}, -\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1,0,-1$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p-2)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(p-2)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-2)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R\bar{3}m$ (166) $\quad$ $\langle 2;\ (4;\ 7)+(2u,2u,2u)\rangle$ $\quad$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations

$p>4;\ 0\le u<p$ $\quad$ u,u,u

p conjugate subgroups for prime $p\equiv 2 \pmod 3$

[p] $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}+(p-1)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p+2)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p-1)\mathbf{b}+(p+2)\mathbf{c}\big)$

$R\bar{3}m$ (166) $\quad$ $\langle 2;\ (4;\ 7)+(2u,2u,2u)\rangle$ $\quad$ $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations

$p>6;\ 0\le u<p$ $\quad$ u,u,u

p conjugate subgroups for prime $p\equiv 1 \pmod 3$

[p^2] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R\bar{3}m$ (166) $\quad$ $\langle 2+(u+v,-2u+v,u-2v);$ $\quad$ $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations

$4+(u-v,-2u+2v,u-v);\ 7+(2u,-2u+2v,-2v)\rangle$ $\quad$ $u,-u+v,-v$

$p>1;\ 0\le u<p;\ 0\le v<p$

p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$

[p^2] $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}+(1-p)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((1-p)\mathbf{a}+(2p+1)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-p)\mathbf{a}+(1-p)\mathbf{b}+(2p+1)\mathbf{c}\big)$

$R\bar{3}m$ (166) $\quad$ $\langle 2+(u+v,-2u+v,u-2v);$ $\quad$ $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}\ldots$, see lattice relations

$4+(u-v,-2u+2v,u-v);\ 7+(2u,-2u+2v,-2v)\rangle$ $\quad$ $u,-u+v,-v$

$p>6;\ 0\le u<p;\ 0\le v<p$

p^2 conjugate subgroups for prime $p\equiv 1 \pmod 3$

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International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 167, pp. 314–316.

$R\bar{3}c$ No. 167 $R\bar{3}2/c$ D_{3d}^{6}

HEXAGONAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$

36	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $R3c$ (161)	(1; 2; 3; 10; 11; 12)+		
[2] $R32$ (155)	(1; 2; 3; 4; 5; 6)+		$0,0,1/4$
[2] $R\bar{3}1$ (148, $R\bar{3}$)	(1; 2; 3; 7; 8; 9)+		
{ [3] $R12/c$ (15, $C12/c1$)	(1; 4; 7; 10)+	$1/3(-\mathbf{a}+\mathbf{b}-2\mathbf{c}),-\mathbf{a}-\mathbf{b},\mathbf{c}$	
{ [3] $R12/c$ (15, $C12/c1$)	(1; 5; 7; 11)+	$1/3(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}),\mathbf{a},\mathbf{c}$	
{ [3] $R12/c$ (15, $C12/c1$)	(1; 6; 7; 12)+	$1/3(2\mathbf{a}+\mathbf{b}-2\mathbf{c}),\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$		$1/3,2/3,2/3$
{ [3] $P\bar{3}c1$ (165)	1; 2; 3; 10; 11; 12; (4; 5; 6; 7; 8; 9) + $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$		$2/3,1/3,1/3$

- **Enlarged unit cell**

[4] $\mathbf{a}'=-2\mathbf{b}$, $\mathbf{b}'=2\mathbf{a}+2\mathbf{b}$

{ $R\bar{3}c$ (167)	$\langle 2;\ 4;\ 7\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $R\bar{3}c$ (167)	$\langle (2;\ 4)+(1,-1,0);\ 7+(2,0,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $R\bar{3}c$ (167)	$\langle 2+(1,2,0);\ 4+(-1,1,0);\ 7+(0,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $R\bar{3}c$ (167)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$-2\mathbf{b},2\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,2u)\rangle$ $p>4$; $0\leq u<p$ p conjugate subgroups for prime $p\equiv 5 \pmod 6$	$-\mathbf{b},\mathbf{a}+\mathbf{b},p\mathbf{c}$	$0,0,u$
$R\bar{3}c$ (167)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,2u)\rangle$ $p>6$; $0\leq u<p$ p conjugate subgroups for prime $p\equiv 1 \pmod 6$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=-p\mathbf{b}$, $\mathbf{b}'=p\mathbf{a}+p\mathbf{b}$

$R\bar{3}c$ (167)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);$ $7+(2u,2v,0)\rangle$ $p>1$; $0\leq u<p$; $0\leq v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$-p\mathbf{b},p\mathbf{a}+p\mathbf{b},\mathbf{c}$	$u,v,0$

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$R\bar{3}c$ (167)	$\langle 2+(u+v,-u+2v,0);\ 4+(u-v,-u+v,0);$ $7+(2u,2v,0)\rangle$ $p>6$; $0\leq u<p$; $0\leq v<p$ p^2 conjugate subgroups for prime $p\equiv 1 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$, $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$, $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P\bar{3}1c$ (163); [2] $\mathbf{a}'=-\mathbf{a}$, $\mathbf{b}'=-\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $R\bar{3}m$ (166)

RHOMBOHEDRAL AXES

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	f	1	(1) x,y,z	(2) z,x,y	(3) y,z,x
			(4) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(5) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$
			(10) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(11) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(12) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $R3c$ (161)	1; 2; 3; 10; 11; 12		
[2] $R32$ (155)	1; 2; 3; 4; 5; 6		1/4, 1/4, 1/4
[2] $R\bar{3}1$ (148, $R\bar{3}$)	1; 2; 3; 7; 8; 9		
{ [3] $R12/c$ (15, $C12/c1$)	1; 4; 7; 10	$-\mathbf{a}-\mathbf{c},-\mathbf{a}+\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ [3] $R12/c$ (15, $C12/c1$)	1; 5; 7; 11	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ [3] $R12/c$ (15, $C12/c1$)	1; 6; 7; 12	$-\mathbf{b}-\mathbf{c},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none

- **Enlarged unit cell**

[3] $\mathbf{a}'=\mathbf{a}-\mathbf{b},\ \mathbf{b}'=\mathbf{b}-\mathbf{c},\ \mathbf{c}'=\mathbf{a}+\mathbf{b}+\mathbf{c}$

{ $P\bar{3}c1$ (165)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ $P\bar{3}c1$ (165)	$\langle 2+(1,-1,0);\ 4+(1,0,1);\ 7+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	1,0,0
{ $P\bar{3}c1$ (165)	$\langle 2+(1,0,-1);\ 4+(1,2,1);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	1,1,0

[4] $\mathbf{a}'=\mathbf{a}-\mathbf{b}+\mathbf{c},\ \mathbf{b}'=\mathbf{a}+\mathbf{b}-\mathbf{c},\ \mathbf{c}'=-\mathbf{a}+\mathbf{b}+\mathbf{c}$

{ $R\bar{3}c$ (167)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ $R\bar{3}c$ (167)	$\langle (2;\ 4)+(1,-2,1);\ 7+(2,-2,0)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	1,−1,0
{ $R\bar{3}c$ (167)	$\langle 2+(1,1,-2);\ 4+(-1,2,-1);\ 7+(0,2,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	0,1,−1
{ $R\bar{3}c$ (167)	$\langle 4;\ 2+(2,-1,-1);\ 7+(2,0,-2)\rangle$	$\mathbf{a}-\mathbf{b}+\mathbf{c},\mathbf{a}+\mathbf{b}-\mathbf{c},-\mathbf{a}+\mathbf{b}+\mathbf{c}$	1,0,−1

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p-2)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(p-2)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-2)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R\bar{3}c$ (167) $\langle 2;\ 4+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u);$ $7+(2u,2u,2u)\rangle$ $\quad \mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations $\quad u,u,u$
$p>4;\ 0\leq u<p$
p conjugate subgroups for prime $p\equiv 5 \pmod 6$

[p] $\mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}+(p-1)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p+2)\mathbf{b}+(p-1)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((p-1)\mathbf{a}+(p-1)\mathbf{b}+(p+2)\mathbf{c}\big)$

$R\bar{3}c$ (167) $\langle 2;\ 4+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2u);$ $7+(2u,2u,2u)\rangle$ $\quad \mathbf{a}'=\frac{1}{3}\big((p+2)\mathbf{a}\ldots$, see lattice relations $\quad u,u,u$
$p>6;\ 0\leq u<p$
p conjugate subgroups for prime $p\equiv 1 \pmod 6$

[p^2] $\mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}+(1-2p)\mathbf{b}+(p+1)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((p+1)\mathbf{a}+(p+1)\mathbf{b}+(1-2p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-2p)\mathbf{a}+(p+1)\mathbf{b}+(p+1)\mathbf{c}\big)$

$R\bar{3}c$ (167) $\langle 2+(u+v,-2u+v,u-2v);$ $\quad \mathbf{a}'=\frac{1}{3}\big((p+1)\mathbf{a}\ldots$, see lattice relations
$4+(u-v,-2u+2v,u-v);$ $\quad u,-u+v,-v$
$7+(2u,-2u+2v,-2v)\rangle$
$p>1;\ 0\leq u<p;\ 0\leq v<p$
p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$

[p^2] $\mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}+(1-p)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{b}'=\frac{1}{3}\big((1-p)\mathbf{a}+(2p+1)\mathbf{b}+(1-p)\mathbf{c}\big),\ \mathbf{c}'=\frac{1}{3}\big((1-p)\mathbf{a}+(1-p)\mathbf{b}+(2p+1)\mathbf{c}\big)$

$R\bar{3}c$ (167) $\langle 2+(u+v,-2u+v,u-2v);$ $\quad \mathbf{a}'=\frac{1}{3}\big((2p+1)\mathbf{a}\ldots$, see lattice relations
$4+(u-v,-2u+2v,u-v);$ $\quad u,-u+v,-v$
$7+(2u,-2u+2v,-2v)\rangle$
$p>6;\ p\equiv 1 \pmod 3;\ 0\leq u<p;\ 0\leq v<p$
p^2 conjugate subgroups for prime $p\equiv 1 \pmod 3$

I Minimal *translationengleiche* supergroups

[4] $Pn\bar{3}n$ (222); [4] $Pm\bar{3}n$ (223); [4] $Fm\bar{3}c$ (226); [4] $Fd\bar{3}c$ (228); [4] $Ia\bar{3}d$ (230)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c}),\ \mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c}),\ \mathbf{c}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ $P\bar{3}1c$ (163);
[2] $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\ \mathbf{b}' = \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\ \mathbf{c}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$ $R\bar{3}m$ (166)

C_6^1 $P6$ No. 168 $P6$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$

I Maximal *translationengleiche* subgroups

[2] $P3$ (143)	1; 2; 3
[3] $P2$ (3, $P112$)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_3$ (173)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6$ (168)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
$P6_4$ (172)	$\langle 4;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6_2$ (171)	$\langle 4;\ 2+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6$ (168)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6$ (168, $P6$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6$ (168, $P6$)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H6$ (168, $P6$)	$\langle 2+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6$ (168)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6$ (168)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P6$ (168)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P6$ (168)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6$ (168)	$\langle 2;\ 4\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6$ (168)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2$ (mod 3)	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2+qr$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P6$ (168)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6/m$ (175); [2] $P622$ (177); [2] $P6mm$ (183); [2] $P6cc$ (184)

II Minimal non-isomorphic *klassengleiche* supergroups none

$P6_1$ No. 169 $P6_1$ C_6^2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	a	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$

I Maximal *translationengleiche* subgroups

[2] $P3_1$ (144) 1; 2; 3
[3] $P2_1$ (4, $P112_1$) 1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b}$

$H6_1$ (169, $P6_1$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6_1$ (169, $P6_1$)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H6_1$ (169, $P6_1$)	$\langle 2+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$

[4] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$

$P6_1$ (169)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6_1$ (169)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P6_1$ (169)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P6_1$ (169)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$

$P6_5$ (170)	$\langle 2+(0,0,\frac{2p}{3}-\frac{1}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>4;\ p\equiv 5 \pmod 6$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P6_1$ (169)	$\langle 2+(0,0,\frac{p}{3}-\frac{1}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>6;\ p\equiv 1 \pmod 6$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	

[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$

$P6_1$ (169)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

[$p=q^2+r^2+qr$] $\mathbf{a}' = q\mathbf{a}-r\mathbf{b},\ \mathbf{b}' = r\mathbf{a}+(q+r)\mathbf{b}$

$P6_1$ (169)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6_122$ (178)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P6_2$ (171); [3] $\mathbf{c}' = \frac{1}{3}\mathbf{c}$ $P6_3$ (173)

C_6^3 $P6_5$ No. 170 $P6_5$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	*a*	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$

I Maximal *translationengleiche* subgroups

[2] $P3_2$ (145)	1; 2; 3
[3] $P2_1$ (4, $P112_1$)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_5$ (170, $P6_5$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6_5$ (170, $P6_5$)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6_5$ (170, $P6_5$)	$\langle 2+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_5$ (170)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_5$ (170)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_5$ (170)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_5$ (170)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6_5$ (170)	$\langle 2+(0,0,\frac{2p}{3}-\frac{2}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>6;\ p\equiv 1\ (\mathrm{mod}\ 6)$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P6_1$ (169)	$\langle 2+(0,0,\frac{p}{3}-\frac{2}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>4;\ p\equiv 5\ (\mathrm{mod}\ 6)$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_5$ (170)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2\ (\mathrm{mod}\ 3)$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2+qr]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P6_5$ (170)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6_522$ (179)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6_4$ (172); [3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P6_3$ (173)

$P6_2$ No. 171 $P6_2$ C_6^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates
6 c 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{2}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$ (4) $\bar{x},\bar{y},z$ (5) $y,\bar{x}+y,z+\frac{2}{3}$ (6) $x-y,x,z+\frac{1}{3}$

I Maximal *translationengleiche* subgroups

[2] $P3_2$ (145)	1; 2; 3
[3] $P2$ (3, $P112$)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_4$ (172)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_1$ (169)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_2$ (171, $P6_2$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6_2$ (171, $P6_2$)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6_2$ (171, $P6_2$)	$\langle 2+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_2$ (171)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_2$ (171)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_2$ (171)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_2$ (171)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6_4$ (172)	$\langle 4;\ 2+(0,0,\frac{p}{3}-\frac{2}{3})\rangle$ $p>1;\ p\equiv 2 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P6_2$ (171)	$\langle 4;\ 2+(0,0,\frac{2p}{3}-\frac{2}{3})\rangle$ $p>6;\ p\equiv 1 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_2$ (171)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2+qr]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P6_2$ (171)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6_222$ (180)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P6$ (168)

C_6^5 $P6_4$ No. 172 $P6_4$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{1}{3}$	(6) $x-y,x,z+\frac{2}{3}$

I Maximal *translationengleiche* subgroups

[2] $P3_1$ (144)	1; 2; 3
[3] $P2$ (3, $P112$)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_2$ (171)	$\langle 4;\ 2+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_5$ (170)	$\langle (2;\ 4)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6_4$ (172, $P6_4$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6_4$ (172, $P6_4$)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,0,0
$H6_4$ (172, $P6_4$)	$\langle 2+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	2,0,0
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6_4$ (172)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6_4$ (172)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,0,0
$P6_4$ (172)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	0,1,0
$P6_4$ (172)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,1,0

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6_4$ (172)	$\langle 4;\ 2+(0,0,\frac{p}{3}-\frac{1}{3})\rangle$ $p>6;\ p\equiv 1 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$P6_2$ (171)	$\langle 4;\ 2+(0,0,\frac{2p}{3}-\frac{1}{3})\rangle$ $p>1;\ p\equiv 2 \pmod 3$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_4$ (172)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2+qr]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P6_4$ (172)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6_422$ (181)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P6$ (168)

$P6_3$ No. 173 $P6_3$ C_6^6

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P3$ (143)	1; 2; 3
[3] $P2_1$ (4, $P112_1$)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P6_3$ (173)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6_5$ (170)	$\langle 2+(0,0,2);\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6_1$ (169)	$\langle (2;\ 4)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_3$ (173, $P6_3$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6_3$ (173, $P6_3$)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,0,0
{ $H6_3$ (173, $P6_3$)	$\langle 2+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	2,0,0
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_3$ (173)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_3$ (173)	$\langle 2+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,0,0
{ $P6_3$ (173)	$\langle 2+(1,2,0);\ 4+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	0,1,0
{ $P6_3$ (173)	$\langle 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,1,0

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6_3$ (173)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_3$ (173)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
$[p=q^2+r^2+qr]$ $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P6_3$ (173)	$\langle 2+(u,-u,0);\ 4+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6_3/m$ (176); [2] $P6_322$ (182); [2] $P6_3cm$ (185); [2] $P6_3mc$ (186)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6$ (168)

C_{3h}^{1} $P\bar{6}$ No. 174 $P\bar{6}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P3$ (143)	1; 2; 3
[3] Pm (6, $P11m$)	1; 4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}' = 2\mathbf{c}$			
$P\bar{6}$ (174)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{6}$ (174)	$\langle 2;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}' = 3\mathbf{c}$			
$P\bar{6}$ (174)	$\langle 2;\ 4\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{6}$ (174)	$\langle 2;\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{6}$ (174)	$\langle 2;\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}' = 3\mathbf{a},\ \mathbf{b}' = 3\mathbf{b}$			
$H\bar{6}$ (174, $P\bar{6}$)	$\langle 2;\ 4\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H\bar{6}$ (174, $P\bar{6}$)	$\langle 4;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H\bar{6}$ (174, $P\bar{6}$)	$\langle 4;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
[4] $\mathbf{a}' = 2\mathbf{a},\ \mathbf{b}' = 2\mathbf{b}$			
$P\bar{6}$ (174)	$\langle 2;\ 4\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P\bar{6}$ (174)	$\langle 4;\ 2+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{6}$ (174)	$\langle 4;\ 2+(1,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P\bar{6}$ (174)	$\langle 4;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}' = p\mathbf{c}$			
$P\bar{6}$ (174)	$\langle 2;\ 4+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P\bar{6}$ (174)	$\langle 4;\ 2+(u+v,-u+2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2+qr$] $\mathbf{a}' = q\mathbf{a}-r\mathbf{b},\ \mathbf{b}' = r\mathbf{a}+(q+r)\mathbf{b}$			
$P\bar{6}$ (174)	$\langle 4;\ 2+(u,-u,0)\rangle$ $q>0;\ r>0;\ p>6;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6/m$ (175); [2] $P6_3/m$ (176); [2] $P\bar{6}m2$ (187); [2] $P\bar{6}c2$ (188); [2] $P\bar{6}2m$ (189); [2] $P\bar{6}2c$ (190)

II Minimal non-isomorphic *klassengleiche* supergroups none

$P6/m$ No. 175 $P6/m$ C_{6h}^{1}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $x,y,\bar{z}$	(11) $\bar{y},x-y,\bar{z}$	(12) $\bar{x}+y,\bar{x},\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}$ (174)	1; 2; 3; 10; 11; 12
[2] $P6$ (168)	1; 2; 3; 4; 5; 6
[2] $P\bar{3}$ (147)	1; 2; 3; 7; 8; 9
[3] $P2/m$ (10, $P112/m$)	1; 4; 7; 10

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_3/m$ (176)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_3/m$ (176)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P6/m$ (175)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6/m$ (175)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P6/m$ (175)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6/m$ (175)	$\langle 2;\ 4;\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P6/m$ (175)	$\langle 2;\ 4;\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6/m$ (175, $P6/m$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6/m$ (175, $P6/m$)	$\langle 2+(1,-1,0);\ (4;\ 7)+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H6/m$ (175, $P6/m$)	$\langle 2+(2,-2,0);\ (4;\ 7)+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6/m$ (175)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6/m$ (175)	$\langle 2+(1,-1,0);\ (4;\ 7)+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P6/m$ (175)	$\langle 2+(1,2,0);\ (4;\ 7)+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P6/m$ (175)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6/m$ (175)	$\langle 2;\ 4;\ 7+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6/m$ (175)	$\langle 2+(u+v,-u+2v,0);\ (4;\ 7)+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2 \pmod 3$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2+qr$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P6/m$ (175)	$\langle 2+(u,-u,0);\ (4;\ 7)+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191); [2] $P6/mcc$ (192)

II Minimal non-isomorphic *klassengleiche* supergroups none

C_{6h}^2 $P6_3/m$ No. 176 $P6_3/m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$
			(10) $x,y,\bar{z}+\frac{1}{2}$	(11) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(12) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}$ (174)	1; 2; 3; 10; 11; 12		$0,0,1/4$
[2] $P6_3$ (173)	1; 2; 3; 4; 5; 6		
[2] $P\bar{3}$ (147)	1; 2; 3; 7; 8; 9		
[3] $P2_1/m$ (11, $P112_1/m$)	1; 4; 7; 10		

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P6_3/m$ (176)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6_3/m$ (176)	$\langle 2;\ 4+(0,0,1);\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P6_3/m$ (176)	$\langle 2;\ 4+(0,0,1);\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6_3/m$ (176, $P6_3/m$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6_3/m$ (176, $P6_3/m$)	$\langle 2+(1,-1,0);\ (4;\ 7)+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H6_3/m$ (176, $P6_3/m$)	$\langle 2+(2,-2,0);\ (4;\ 7)+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6_3/m$ (176)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6_3/m$ (176)	$\langle 2+(1,-1,0);\ (4;\ 7)+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P6_3/m$ (176)	$\langle 2+(1,2,0);\ (4;\ 7)+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P6_3/m$ (176)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6_3/m$ (176)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2});\ 7+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_3/m$ (176)	$\langle 2+(u+v,-u+2v,0);\ (4;\ 7)+(2u,2v,0)\rangle$ $p>1;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for prime $p\equiv 2\ (\mathrm{mod}\ 3)$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$
[$p=q^2+r^2+qr$] $\mathbf{a}'=q\mathbf{a}-r\mathbf{b},\ \mathbf{b}'=r\mathbf{a}+(q+r)\mathbf{b}$			
$P6_3/m$ (176)	$\langle 2+(u,-u,0);\ (4;\ 7)+(2u,0,0)\rangle$ $q>0;\ r>0;\ p>2;\ 0\le u<p$ p conjugate subgroups for each pair of q and r	$q\mathbf{a}-r\mathbf{b},r\mathbf{a}+(q+r)\mathbf{b},\mathbf{c}$	$u,0,0$

I Minimal *translationengleiche* supergroups

[2] $P6_3/mcm$ (193); [2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6/m$ (175)

$P622$ No. 177 $P622$ D_6^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	n	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P611$ (168, $P6$)	1; 2; 3; 4; 5; 6		
[2] $P321$ (150)	1; 2; 3; 7; 8; 9		
[2] $P312$ (149)	1; 2; 3; 10; 11; 12		
{ [3] $P222$ (21, $C222$)	1; 4; 7; 10	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	
{ [3] $P222$ (21, $C222$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
{ [3] $P222$ (21, $C222$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_322$ (182)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_322$ (182)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P622$ (177)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P622$ (177)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P6_422$ (181)	$\langle 4;\ (2;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P6_422$ (181)	$\langle 4;\ 2+(0,0,1);\ 7+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P6_422$ (181)	$\langle 4;\ 2+(0,0,1);\ 7+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
{ $P6_222$ (180)	$\langle 4;\ (2;\ 7)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P6_222$ (180)	$\langle 4;\ 2+(0,0,2);\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P6_222$ (180)	$\langle 4;\ 2+(0,0,2);\ 7+(0,0,6)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
{ $P622$ (177)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P622$ (177)	$\langle 2;\ 4;\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P622$ (177)	$\langle 2;\ 4;\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H622$ (177, $P622$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H622$ (177, $P622$)	$\langle (2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H622$ (177, $P622$)	$\langle (2;\ 7)+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P622$ (177)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P622$ (177)	$\langle (2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P622$ (177)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P622$ (177)	$\langle 7;\ 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P622$ (177)	$\langle 2;\ 4;\ 7+(0,0,2u)\rangle$ $p>2;\ 0\leq u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P622$ (177)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191); [2] $P6/mcc$ (192)

II Minimal non-isomorphic *klassengleiche* supergroups none

D_6^2 $P6_122$ No. 178 $P6_122$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
12 c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$
	(7) $y,x,\bar{z}+\frac{1}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$
	(10) $\bar{y},\bar{x},\bar{z}+\frac{5}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{6}$

I Maximal *translationengleiche* subgroups

[2] $P6_111$ (169, $P6_1$)	1; 2; 3; 4; 5; 6		
[2] $P3_121$ (152)	1; 2; 3; 7; 8; 9		0,0,1/6
[2] $P3_112$ (151)	1; 2; 3; 10; 11; 12		0,0,1/12
{ [3] $P2_122$ (20, $C222_1$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	0,0,5/12
{ [3] $P2_122$ (20, $C222_1$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	0,0,3/4
{ [3] $P2_122$ (20, $C222_1$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	0,0,1/12

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=3\mathbf{b}$

{ $H6_122$ (178, $P6_122$)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	0,0,5/12
{ $H6_122$ (178, $P6_122$)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,-1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,0,5/12
{ $H6_122$ (178, $P6_122$)	$\langle 2+(2,-2,0);\ 4+(4,0,0);\ 7+(2,-2,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	2,0,5/12

[4] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$

{ $P6_122$ (178)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_122$ (178)	$\langle (2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,0,0
{ $P6_122$ (178)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	0,1,0
{ $P6_122$ (178)	$\langle 7;\ 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,1,0

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$

$P6_522$ (179)	$\langle 2+(0,0,\frac{2p}{3}-\frac{1}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2});$ $7+(0,0,\frac{2p}{3}-\frac{1}{3}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 5$ (mod 6)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P6_122$ (178)	$\langle 2+(0,0,\frac{p}{3}-\frac{1}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2});$ $7+(0,0,\frac{p}{3}-\frac{1}{3}+2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 6)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

$[p^2]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$P6_122$ (178)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6_222$ (180); [3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P6_322$ (182)

$P6_522$ No. 179 $P6_522$ D_6^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

12 c 1

(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$
(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$
(7) $y,x,\bar{z}+\frac{2}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$
(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{5}{6}$

I Maximal *translationengleiche* subgroups

[2] $P6_511$ (170, $P6_5$)	1; 2; 3; 4; 5; 6		
[2] $P3_221$ (154)	1; 2; 3; 7; 8; 9		$0,0,1/3$
[2] $P3_212$ (153)	1; 2; 3; 10; 11; 12		$0,0,5/12$
{ [3] $P2_122$ (20, $C222_1$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,0,1/12$
{ [3] $P2_122$ (20, $C222_1$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	$0,0,3/4$
{ [3] $P2_122$ (20, $C222_1$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	$0,0,5/12$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=3\mathbf{b}$

{ $H6_522$ (179, $P6_522$)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,7/12$
{ $H6_522$ (179, $P6_522$)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,-1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,7/12$
{ $H6_522$ (179, $P6_522$)	$\langle 2+(2,-2,0);\ 4+(4,0,0);\ 7+(2,-2,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,7/12$

[4] $\mathbf{a}'=2\mathbf{a}$, $\mathbf{b}'=2\mathbf{b}$

{ $P6_522$ (179)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_522$ (179)	$\langle (2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_522$ (179)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_522$ (179)	$\langle 7;\ 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$

$P6_522$ (179)	$\langle 2+(0,0,\frac{2p}{3}-\frac{2}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2});$ $7+(0,0,\frac{2p}{3}-\frac{2}{3}+2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 6)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P6_122$ (178)	$\langle 2+(0,0,\frac{p}{3}-\frac{2}{3});\ 4+(0,0,\frac{p}{2}-\frac{1}{2});$ $7+(0,0,\frac{p}{3}-\frac{2}{3}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 5$ (mod 6)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$

[p^2] $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$

$P6_522$ (179)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6_422$ (181); [3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P6_322$ (182)

D_6^4 $P6_222$ No. 180 $P6_222$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
12 k 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{2}{3}$	(6) $x-y,x,z+\frac{1}{3}$
	(7) $y,x,\bar{z}+\frac{2}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$
	(10) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}+\frac{1}{3}$

I Maximal *translationengleiche* subgroups

[2] $P6_211$ (171, $P6_2$)	1; 2; 3; 4; 5; 6		
[2] $P3_221$ (154)	1; 2; 3; 7; 8; 9		0,0,1/3
[2] $P3_212$ (153)	1; 2; 3; 10; 11; 12		0,0,1/6
{ [3] $P222$ (21, $C222$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	0,0,1/3
{ [3] $P222$ (21, $C222$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
{ [3] $P222$ (21, $C222$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	0,0,2/3

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_422$ (181)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_422$ (181)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	0,0,1/2
$P6_122$ (178)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_122$ (178)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	0,0,1/2
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_222$ (180, $P6_222$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	0,0,1/3
{ $H6_222$ (180, $P6_222$)	$\langle(2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,0,1/3
{ $H6_222$ (180, $P6_222$)	$\langle(2;\ 7)+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	2,0,1/3
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_222$ (180)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_222$ (180)	$\langle(2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,0,0
{ $P6_222$ (180)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	0,1,0
{ $P6_222$ (180)	$\langle 7;\ 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,1,0

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6_422$ (181)	$\langle 4;\ 2+(0,0,\frac{p}{3}-\frac{2}{3});\ 7+(0,0,\frac{p}{3}-\frac{2}{3}+2u)\rangle$ $p>4$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 2$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P6_222$ (180)	$\langle 4;\ 2+(0,0,\frac{2p}{3}-\frac{2}{3});\ 7+(0,0,\frac{2p}{3}-\frac{2}{3}+2u)\rangle$ $p>6$; $0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_222$ (180)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1$; $p\ne 3$; $0\le u<p$; $0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P622$ (177)

$P6_422$ No. 181 $P6_422$ D_6^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
12 k 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{1}{3}$	(6) $x-y,x,z+\frac{2}{3}$
	(7) $y,x,\bar{z}+\frac{1}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$
	(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}+\frac{2}{3}$

I Maximal *translationengleiche* subgroups

[2] $P6_411$ (172, $P6_4$)	1; 2; 3; 4; 5; 6		
[2] $P3_121$ (152)	1; 2; 3; 7; 8; 9		$0,0,1/6$
[2] $P3_112$ (151)	1; 2; 3; 10; 11; 12		$0,0,1/3$
{ [3] $P222$ (21, $C222$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,0,2/3$
{ [3] $P222$ (21, $C222$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
{ [3] $P222$ (21, $C222$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	$0,0,1/3$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_222$ (180)	$\langle 4;\ (2;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_222$ (180)	$\langle 4;\ 2+(0,0,1);\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P6_522$ (179)	$\langle 7;\ (2;\ 4)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P6_522$ (179)	$\langle (2;\ 4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_422$ (181, $P6_422$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,1/6$
{ $H6_422$ (181, $P6_422$)	$\langle (2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,1/6$
{ $H6_422$ (181, $P6_422$)	$\langle (2;\ 7)+(2,-2,0);\ 4+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,1/6$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_422$ (181)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_422$ (181)	$\langle (2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_422$ (181)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_422$ (181)	$\langle 7;\ 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6_422$ (181)	$\langle 4;\ 2+(0,0,\frac{p}{3}-\frac{1}{3});\ 7+(0,0,\frac{p}{3}-\frac{1}{3}+2u)\rangle$ $p>6;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 1$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$P6_222$ (180)	$\langle 4;\ 2+(0,0,\frac{2p}{3}-\frac{1}{3});\ 7+(0,0,\frac{2p}{3}-\frac{1}{3}+2u)\rangle$ $p>4;\ 0\le u<p$ p conjugate subgroups for prime $p\equiv 2$ (mod 3)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_422$ (181)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[3] $\mathbf{c}'=\frac{1}{3}\mathbf{c}$ $P622$ (177)

D_6^6 $P6_322$ No. 182 $P6_322$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	*i*	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P6_311$ (173, $P6_3$)	1; 2; 3; 4; 5; 6		
[2] $P321$ (150)	1; 2; 3; 7; 8; 9		
[2] $P312$ (149)	1; 2; 3; 10; 11; 12		$0,0,1/4$
[3] $P2_122$ (20, $C222_1$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$0,0,1/4$
[3] $P2_122$ (20, $C222_1$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	$0,0,1/4$
[3] $P2_122$ (20, $C222_1$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	$0,0,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P6_322$ (182)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6_322$ (182)	$\langle 2;\ 4+(0,0,1);\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P6_322$ (182)	$\langle 2;\ 4+(0,0,1);\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
$P6_522$ (179)	$\langle (2;\ 7)+(0,0,2);\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6_522$ (179)	$\langle 2+(0,0,2);\ 4+(0,0,1);\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P6_522$ (179)	$\langle 2+(0,0,2);\ 4+(0,0,1);\ 7+(0,0,6)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
$P6_122$ (178)	$\langle (2;\ 4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6_122$ (178)	$\langle (2;\ 4)+(0,0,1);\ 7+(0,0,3)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P6_122$ (178)	$\langle (2;\ 4)+(0,0,1);\ 7+(0,0,5)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6_322$ (182, $P6_322$)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$0,0,1/4$
$H6_322$ (182, $P6_322$)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,-1,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,1/4$
$H6_322$ (182, $P6_322$)	$\langle 2+(2,-2,0);\ 4+(4,0,0);\ 7+(2,-2,1)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,1/4$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6_322$ (182)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6_322$ (182)	$\langle (2;\ 7)+(1,-1,0);\ 4+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P6_322$ (182)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P6_322$ (182)	$\langle 7;\ 2+(2,1,0);\ 4+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6_322$ (182)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2});\ 7+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_322$ (182)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_3/mcm$ (193); [2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P622$ (177)

$P6mm$ No. 183 $P6mm$ C_{6v}^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$

I Maximal *translationengleiche* subgroups

[2] $P611$ (168, $P6$)	1; 2; 3; 4; 5; 6		
[2] $P31m$ (157)	1; 2; 3; 10; 11; 12		
[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9		
[3] $P2mm$ (35, $Cmm2$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $P2mm$ (35, $Cmm2$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
[3] $P2mm$ (35, $Cmm2$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_3mc$ (186)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_3cm$ (185)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6cc$ (184)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6mm$ (183)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
[3] $\mathbf{c}'=3\mathbf{c}$			
$P6mm$ (183)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6mm$ (183, $P6mm$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6mm$ (183, $P6mm$)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H6mm$ (183, $P6mm$)	$\langle 2+(2,-2,0);\ 4+(4,0,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6mm$ (183)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6mm$ (183)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P6mm$ (183)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P6mm$ (183)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6mm$ (183)	$\langle 2;\ 4;\ 7\rangle$ $p>1$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6mm$ (183)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191)

II Minimal non-isomorphic *klassengleiche* supergroups none

C_{6v}^{2} $P6cc$ No. 184 $P6cc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$
			(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P611$ (168, $P6$)	1; 2; 3; 4; 5; 6	
[2] $P31c$ (159)	1; 2; 3; 10; 11; 12	
[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9	
{ [3] $P2cc$ (37, $Ccc2$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$
{ [3] $P2cc$ (37, $Ccc2$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$
{ [3] $P2cc$ (37, $Ccc2$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P6cc$ (184)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6cc$ (184, $P6cc$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6cc$ (184, $P6cc$)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6cc$ (184, $P6cc$)	$\langle 2+(2,-2,0);\ 4+(4,0,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6cc$ (184)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6cc$ (184)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6cc$ (184)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6cc$ (184)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6cc$ (184)	$\langle 2;\ 4;\ 7+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6cc$ (184)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mcc$ (192)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6mm$ (183)

$P6_3cm$ No. 185 $P6_3cm$ C_{6v}^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
			(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$

I Maximal *translationengleiche* subgroups

[2] $P6_311$ (173, $P6_3$)	1; 2; 3; 4; 5; 6	
[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9	
[2] $P31m$ (157)	1; 2; 3; 10; 11; 12	
{ [3] $P2_1cm$ (36, $Cmc2_1$)	1; 4; 7; 10	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$
{ [3] $P2_1cm$ (36, $Cmc2_1$)	1; 4; 8; 11	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$
{ [3] $P2_1cm$ (36, $Cmc2_1$)	1; 4; 9; 12	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P6_3cm$ (185)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_3cm$ (186, $P6_3mc$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6_3cm$ (186, $P6_3mc$)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6_3cm$ (186, $P6_3mc$)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_3cm$ (185)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_3cm$ (185)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_3cm$ (185)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_3cm$ (185)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6_3cm$ (185)	$\langle 2;\ (4;\ 7)+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_3cm$ (185)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_3/mcm$ (193)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H6_3cm$ (186, $P6_3mc$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6mm$ (183)

C_{6v}^4 $P6_3mc$ No. 186 $P6_3mc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
12 *d* 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
	(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$
	(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P6_311$ (173, $P6_3$)	1; 2; 3; 4; 5; 6	
[2] $P31c$ (159)	1; 2; 3; 10; 11; 12	
[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9	
[3] $P2_1mc$ (36, $Cmc2_1$)	1; 4; 7; 10	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$
[3] $P2_1mc$ (36, $Cmc2_1$)	1; 4; 8; 11	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$
[3] $P2_1mc$ (36, $Cmc2_1$)	1; 4; 9; 12	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P6_3mc$ (186)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6_3mc$ (185, $P6_3cm$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6_3mc$ (185, $P6_3cm$)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,0,0
$H6_3mc$ (185, $P6_3cm$)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	1,1,0
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6_3mc$ (186)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6_3mc$ (186)	$\langle 2+(1,-1,0);\ 4+(2,0,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,0,0
$P6_3mc$ (186)	$\langle 2+(1,2,0);\ 4+(0,2,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	0,1,0
$P6_3mc$ (186)	$\langle 2+(2,1,0);\ (4;\ 7)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	1,1,0

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6_3mc$ (186)	$\langle 2;\ 7;\ 4+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$ no conjugate subgroups	$\mathbf{a},\mathbf{b},p\mathbf{c}$	
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_3mc$ (186)	$\langle 2+(u+v,-u+2v,0);\ 4+(2u,2v,0);$ $7+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\leq u<p;\ 0\leq v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H6_3mc$ (185, $P6_3cm$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6mm$ (183)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 187, pp. 336–337.

$P\bar{6}m2$ No. 187 $P\bar{6}m2$ D_{3h}^{1}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	o	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}11$ (174, $P\bar{6}$)	1; 2; 3; 4; 5; 6		
[2] $P3m1$ (156)	1; 2; 3; 7; 8; 9		
[2] $P312$ (149)	1; 2; 3; 10; 11; 12		
[3] $Pmm2$ (38, $Amm2$)	1; 4; 7; 10	$\mathbf{c},-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b}$	
[3] $Pmm2$ (38, $Amm2$)	1; 4; 8; 11	$\mathbf{c},\mathbf{a},\mathbf{a}+2\mathbf{b}$	
[3] $Pmm2$ (38, $Amm2$)	1; 4; 9; 12	$\mathbf{c},\mathbf{b},-2\mathbf{a}-\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{6}c2$ (188)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{6}c2$ (188)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{6}m2$ (187)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{6}m2$ (187)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
$P\bar{6}m2$ (187)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{6}m2$ (187)	$\langle 2;\ 7;\ 4+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{6}m2$ (187)	$\langle 2;\ 7;\ 4+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ 2+(1,-1,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ 2+(1,0,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ (2;\ 7)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ 2+(3,4,0);\ 7+(3,3,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,7/3,0$
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ (2;\ 7)+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ 2+(2,0,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
$H\bar{6}m2$ (189, $P\bar{6}2m$)	$\langle 4;\ 2+(3,-1,0);\ 7+(3,3,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$7/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P\bar{6}m2$ (187)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P\bar{6}m2$ (187)	$\langle 4;\ 2+(1,-1,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{6}m2$ (187)	$\langle 4;\ 2+(1,2,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P\bar{6}m2$ (187)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{6}m2$ (187)	$\langle 2;\ 7;\ 4+(0,0,2u)\rangle$ $p>1;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{6}m2$ (187)	$\langle 4;\ 2+(u+v,-u+2v,0);\ 7+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191); [2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{6}m2$ (189, $P\bar{6}2m$)

- **Decreased unit cell** none

$P\bar{6}c2$ No. 188 $P\bar{6}c2$ D_{3h}^2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
12 *l* 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
	(4) $x,y,\bar{z}+\frac{1}{2}$	(5) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(6) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$
	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$
	(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}11$ (174, $P\bar{6}$)	1; 2; 3; 4; 5; 6		$0,0,1/4$
[2] $P3c1$ (158)	1; 2; 3; 7; 8; 9		
[2] $P312$ (149)	1; 2; 3; 10; 11; 12		
[3] $Pmc2$ (40, $Ama2$)	1; 4; 7; 10	$\mathbf{c},-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b}$	
[3] $Pmc2$ (40, $Ama2$)	1; 4; 8; 11	$\mathbf{c},\mathbf{a},\mathbf{a}+2\mathbf{b}$	
[3] $Pmc2$ (40, $Ama2$)	1; 4; 9; 12	$\mathbf{c},\mathbf{b},-2\mathbf{a}-\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P\bar{6}c2$ (188)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P\bar{6}c2$ (188)	$\langle 2;\ 4+(0,0,3);\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P\bar{6}c2$ (188)	$\langle 2;\ 4+(0,0,5);\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 2+(1,-1,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 7;\ 2+(1,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$-1/3,1/3,0$
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 2+(2,-1,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,1/3,0$
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 2+(3,1,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2/3,4/3,0$
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 7;\ 2+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,-1/3,0$
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 2+(2,3,0);\ 7+(1,1,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1/3,2/3,0$
$H\bar{6}c2$ (190, $P\bar{6}2c$)	$\langle 4;\ 2+(3,2,0);\ 7+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$4/3,2/3,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P\bar{6}c2$ (188)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P\bar{6}c2$ (188)	$\langle 4;\ 2+(1,-1,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P\bar{6}c2$ (188)	$\langle 4;\ 2+(1,2,0);\ 7+(1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P\bar{6}c2$ (188)	$\langle 4;\ 2+(2,1,0);\ 7+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{6}c2$ (188)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{6}c2$ (188)	$\langle 4;\ 2+(u+v,-u+2v,0);\ 7+(u+v,u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mcc$ (192); [2] $P6_3/mcm$ (193)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{6}c2$ (190, $P\bar{6}2c$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{6}m2$ (187)

D_{3h}^{3} $P\bar{6}2m$ No. 189 $P\bar{6}2m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		
12 l 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
	(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$
	(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$
	(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}11$ (174, $P\bar{6}$)	1; 2; 3; 4; 5; 6		
[2] $P31m$ (157)	1; 2; 3; 10; 11; 12		
[2] $P321$ (150)	1; 2; 3; 7; 8; 9		
{ [3] $Pm2m$ (38, $Amm2$)	1; 4; 7; 10	$\mathbf{c},-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b}$	
{ [3] $Pm2m$ (38, $Amm2$)	1; 4; 8; 11	$\mathbf{c},-\mathbf{a}-2\mathbf{b},\mathbf{a}$	
{ [3] $Pm2m$ (38, $Amm2$)	1; 4; 9; 12	$\mathbf{c},2\mathbf{a}+\mathbf{b},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P\bar{6}2c$ (190)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{6}2c$ (190)	$\langle 2;\ 4;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P\bar{6}2m$ (189)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P\bar{6}2m$ (189)	$\langle 2;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{6}2m$ (189)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{6}2m$ (189)	$\langle 2;\ (4;\ 7)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{6}2m$ (189)	$\langle 2;\ (4;\ 7)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H\bar{6}2m$ (187, $P\bar{6}m2$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P\bar{6}2m$ (189)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P\bar{6}2m$ (189)	$\langle 4;\ (2;\ 7)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P\bar{6}2m$ (189)	$\langle 4;\ 2+(1,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P\bar{6}2m$ (189)	$\langle 4;\ 7;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P\bar{6}2m$ (189)	$\langle 2;\ (4;\ 7)+(0,0,2u)\rangle$ $p>1;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{6}2m$ (189)	$\langle 4;\ 2+(u+v,-u+2v,0);\ 7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mmm$ (191); [2] $P6_3/mcm$ (193)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{6}2m$ (187, $P\bar{6}m2$)

- **Decreased unit cell** none

$P\bar{6}2c$ No. 190 $P\bar{6}2c$ D_{3h}^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
12	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $x,y,\bar{z}+\frac{1}{2}$	(5) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(6) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$
			(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}11$ (174, $P\bar{6}$)	1; 2; 3; 4; 5; 6		$0,0,1/4$
[2] $P31c$ (159)	1; 2; 3; 10; 11; 12		
[2] $P321$ (150)	1; 2; 3; 7; 8; 9		
{ [3] $Pm2c$ (40, $Ama2$)	1; 4; 7; 10	$\mathbf{c},-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b}$	
{ [3] $Pm2c$ (40, $Ama2$)	1; 4; 8; 11	$\mathbf{c},-\mathbf{a}-2\mathbf{b},\mathbf{a}$	
{ [3] $Pm2c$ (40, $Ama2$)	1; 4; 9; 12	$\mathbf{c},2\mathbf{a}+\mathbf{b},\mathbf{b}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P\bar{6}2c$ (190)	$\langle 2;\ 7;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P\bar{6}2c$ (190)	$\langle 2;\ 4+(0,0,3);\ 7+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P\bar{6}2c$ (190)	$\langle 2;\ 4+(0,0,5);\ 7+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H\bar{6}2c$ (188, $P\bar{6}c2$)	$\langle 2;\ 4;\ 7\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P\bar{6}2c$ (190)	$\langle 2;\ 4;\ 7\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P\bar{6}2c$ (190)	$\langle 4;\ (2;\ 7)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P\bar{6}2c$ (190)	$\langle 4;\ 2+(1,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P\bar{6}2c$ (190)	$\langle 4;\ 7;\ 2+(2,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P\bar{6}2c$ (190)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 7+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P\bar{6}2c$ (190)	$\langle 4;\ 2+(u+v,-u+2v,0);\ 7+(u-v,-u+v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups

[2] $P6/mcc$ (192); [2] $P6_3/mmc$ (194)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H\bar{6}2c$ (188, $P\bar{6}c2$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{6}2m$ (189)

D_{6h}^1 $P6/m2/m2/m$ No. 191 $P6/mmm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
24	r	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$
			(16) $x,y,\bar{z}$	(17) $\bar{y},x-y,\bar{z}$	(18) $\bar{x}+y,\bar{x},\bar{z}$
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$
			(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}2m$ (189)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24	
[2] $P\bar{6}m2$ (187)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21	
[2] $P6mm$ (183)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24	
[2] $P622$ (177)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12	
[2] $P6/m11$ (175, $P6/m$)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18	
[2] $P\bar{3}m1$ (164)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21	
[2] $P\bar{3}1m$ (162)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24	
{ [3] $Pmmm$ (65, $Cmmm$)	1; 4; 7; 10; 13; 16; 19; 22	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$
{ [3] $Pmmm$ (65, $Cmmm$)	1; 4; 8; 11; 13; 16; 20; 23	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$
{ [3] $Pmmm$ (65, $Cmmm$)	1; 4; 9; 12; 13; 16; 21; 24	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{c}'=2\mathbf{c}$			
$P6_3/mmc$ (194)	$\langle 2;\ 7;\ 13;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_3/mmc$ (194)	$\langle 2;\ (4;\ 7;\ 13)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P6_3/mcm$ (193)	$\langle 2;\ 13;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6_3/mcm$ (193)	$\langle 2;\ 7;\ (4;\ 13)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P6/mcc$ (192)	$\langle 2;\ 4;\ 13;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6/mcc$ (192)	$\langle 2;\ 4;\ 7;\ 13+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
$P6/mmm$ (191)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	
$P6/mmm$ (191)	$\langle 2;\ 4;\ (7;\ 13)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$0,0,1/2$
[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P6/mmm$ (191)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P6/mmm$ (191)	$\langle 2;\ 4;\ (7;\ 13)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P6/mmm$ (191)	$\langle 2;\ 4;\ (7;\ 13)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6/mmm$ (191, $P6/mmm$)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6/mmm$ (191, $P6/mmm$)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6/mmm$ (191, $P6/mmm$)	$\langle (2;\ 7)+(2,-2,0);\ (4;\ 13)+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6/mmm$ (191)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6/mmm$ (191)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6/mmm$ (191)	$\langle 2+(1,2,0);\ (4;\ 13)+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6/mmm$ (191)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}' = p\mathbf{c}$			
$P6/mmm$ (191)	$\langle 2;\ 4;\ (7;\ 13) + (0,0,2u) \rangle$ $p > 2;\ 0 \le u < p$ p conjugate subgroups for the prime p	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b}$			
$P6/mmm$ (191)	$\langle 2 + (u+v, -u+2v, 0);\ (4;\ 13) + (2u, 2v, 0);$ $7 + (u-v, -u+v, 0) \rangle$ $p > 1;\ p \ne 3;\ 0 \le u < p;\ 0 \le v < p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups none

D_{6h}^2 $P6/m2/c2/c$ No. 192 $P6/mcc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates					
24	m	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$
			(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$	(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	(16) $x,y,\bar{z}$	(17) $\bar{y},x-y,\bar{z}$	(18) $\bar{x}+y,\bar{x},\bar{z}$
			(19) $\bar{y},\bar{x},z+\frac{1}{2}$	(20) $\bar{x}+y,y,z+\frac{1}{2}$	(21) $x,x-y,z+\frac{1}{2}$	(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}2c$ (190)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24		$0,0,1/4$
[2] $P\bar{6}c2$ (188)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21		$0,0,1/4$
[2] $P6cc$ (184)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24		
[2] $P622$ (177)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		$0,0,1/4$
[2] $P6/m11$ (175, $P6/m$)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18		
[2] $P\bar{3}c1$ (165)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21		
[2] $P\bar{3}1c$ (163)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24		
[3] $Pmcc$ (66, $Cccm$)	1; 4; 7; 10; 13; 16; 19; 22	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
[3] $Pmcc$ (66, $Cccm$)	1; 4; 8; 11; 13; 16; 20; 23	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
[3] $Pmcc$ (66, $Cccm$)	1; 4; 9; 12; 13; 16; 21; 24	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
$P6/mcc$ (192)	$\langle 2;\ 4;\ 13;\ 7+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
$P6/mcc$ (192)	$\langle 2;\ 4;\ 7+(0,0,3);\ 13+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
$P6/mcc$ (192)	$\langle 2;\ 4;\ 7+(0,0,5);\ 13+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
$H6/mcc$ (192, $P6/mcc$)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
$H6/mcc$ (192, $P6/mcc$)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
$H6/mcc$ (192, $P6/mcc$)	$\langle (2;\ 7)+(2,-2,0);\ (4;\ 13)+(4,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$2,0,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
$P6/mcc$ (192)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
$P6/mcc$ (192)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
$P6/mcc$ (192)	$\langle 2+(1,2,0);\ (4;\ 13)+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
$P6/mcc$ (192)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6/mcc$ (192)	$\langle 2;\ 4;\ 7+(0,0,\frac{p}{2}-\frac{1}{2}+2u);\ 13+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6/mcc$ (192)	$\langle 2+(u+v,-u+2v,0);\ (4;\ 13)+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6/mmm$ (191)

$P6_3/mcm$ No. 193 $P6_3/m2/c2/m$ D_{6h}^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates					
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
			(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$	(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$
			(19) $\bar{y},\bar{x},z+\frac{1}{2}$	(20) $\bar{x}+y,y,z+\frac{1}{2}$	(21) $x,x-y,z+\frac{1}{2}$	(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}2m$ (189)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24		$0,0,1/4$
[2] $P\bar{6}c2$ (188)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21		
[2] $P6_3cm$ (185)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24		
[2] $P6_322$ (182)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		$0,0,1/4$
[2] $P6_3/m11$ (176, $P6_3/m$)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18		
[2] $P\bar{3}c1$ (165)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21		
[2] $P\bar{3}1m$ (162)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24		
{ [3] $Pmcm$ (63, $Cmcm$)	1; 4; 7; 10; 13; 16; 19; 22	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	
{ [3] $Pmcm$ (63, $Cmcm$)	1; 4; 8; 11; 13; 16; 20; 23	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	
{ [3] $Pmcm$ (63, $Cmcm$)	1; 4; 9; 12; 13; 16; 21; 24	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P6_3/mcm$ (193)	$\langle 2;\ 13;\ (4;\ 7)+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P6_3/mcm$ (193)	$\langle 2;\ 4+(0,0,1);\ 7+(0,0,3);\ 13+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P6_3/mcm$ (193)	$\langle 2;\ 4+(0,0,1);\ 7+(0,0,5);\ 13+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_3/mcm$ (194, $P6_3/mmc$)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6_3/mcm$ (194, $P6_3/mmc$)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6_3/mcm$ (194, $P6_3/mmc$)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_3/mcm$ (193)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_3/mcm$ (193)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_3/mcm$ (193)	$\langle 2+(1,2,0);\ (4;\ 13)+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_3/mcm$ (193)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

[p] $\mathbf{c}'=p\mathbf{c}$			
$P6_3/mcm$ (193)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2});\ 7+(0,0,\frac{p}{2}-\frac{1}{2}+2u);$ $13+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
[p^2] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_3/mcm$ (193)	$\langle 2+(u+v,-u+2v,0);\ (4;\ 13)+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\ne 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H6_3/mcm$ (194, $P6_3/mmc$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6/mmm$ (191)

D_{6h}^4 $P6_3/m2/m2/c$ No. 194 $P6_3/mmc$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates					
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$	(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$	(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{6}2c$ (190)	1; 2; 3; 7; 8; 9; 16; 17; 18; 22; 23; 24		
[2] $P\bar{6}m2$ (187)	1; 2; 3; 10; 11; 12; 16; 17; 18; 19; 20; 21		$0,0,1/4$
[2] $P6_3mc$ (186)	1; 2; 3; 4; 5; 6; 19; 20; 21; 22; 23; 24		
[2] $P6_322$ (182)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[2] $P6_3/m11$ (176, $P6_3/m$)	1; 2; 3; 4; 5; 6; 13; 14; 15; 16; 17; 18		
[2] $P\bar{3}m1$ (164)	1; 2; 3; 7; 8; 9; 13; 14; 15; 19; 20; 21		
[2] $P\bar{3}1c$ (163)	1; 2; 3; 10; 11; 12; 13; 14; 15; 22; 23; 24		
{ [3] $Pmmc$ (63, $Cmcm$)	1; 4; 7; 10; 13; 16; 19; 22	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	
{ [3] $Pmmc$ (63, $Cmcm$)	1; 4; 8; 11; 13; 16; 20; 23	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ [3] $Pmmc$ (63, $Cmcm$)	1; 4; 9; 12; 13; 16; 21; 24	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[3] $\mathbf{c}'=3\mathbf{c}$			
{ $P6_3/mmc$ (194)	$\langle 2;\ 7;\ 13;\ 4+(0,0,1)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	
{ $P6_3/mmc$ (194)	$\langle 2;\ 4+(0,0,1);\ (7;\ 13)+(0,0,2)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,1$
{ $P6_3/mmc$ (194)	$\langle 2;\ 4+(0,0,1);\ (7;\ 13)+(0,0,4)\rangle$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$0,0,2$
[3] $\mathbf{a}'=3\mathbf{a},\ \mathbf{b}'=3\mathbf{b}$			
{ $H6_3/mmc$ (193, $P6_3/mcm$)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	
{ $H6_3/mmc$ (193, $P6_3/mcm$)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $H6_3/mmc$ (193, $P6_3/mcm$)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$\mathbf{a}-\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$1,1,0$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b}$			
{ $P6_3/mmc$ (194)	$\langle 2;\ 4;\ 7;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	
{ $P6_3/mmc$ (194)	$\langle (2;\ 7)+(1,-1,0);\ (4;\ 13)+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,0,0$
{ $P6_3/mmc$ (194)	$\langle 2+(1,2,0);\ (4;\ 13)+(0,2,0);\ 7+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$0,1,0$
{ $P6_3/mmc$ (194)	$\langle 7;\ 2+(2,1,0);\ (4;\ 13)+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$1,1,0$

- **Series of maximal isomorphic subgroups**

$[p]$ $\mathbf{c}'=p\mathbf{c}$			
$P6_3/mmc$ (194)	$\langle 2;\ 4+(0,0,\frac{p}{2}-\frac{1}{2});\ (7;\ 13)+(0,0,2u)\rangle$ $p>2;\ 0\le u<p$ p conjugate subgroups for the prime p	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$0,0,u$
$[p^2]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b}$			
$P6_3/mmc$ (194)	$\langle 2+(u+v,-u+2v,0);\ (4;\ 13)+(2u,2v,0);$ $7+(u-v,-u+v,0)\rangle$ $p>1;\ p\neq 3;\ 0\le u<p;\ 0\le v<p$ p^2 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$u,v,0$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[3] $H6_3/mmc$ (193, $P6_3/mcm$)

- **Decreased unit cell**

[2] $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P6/mmm$ (191)

$P23$ No. 195 $P23$ T^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
12	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$

I Maximal *translationengleiche* subgroups

[3] $P21$ (16, $P222$)	1; 2; 3; 4		
{ [4] $P13$ (146, $R3$)	1; 5; 9	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	
{ [4] $P13$ (146, $R3$)	1; 6; 12	$-\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}, -\mathbf{a}+\mathbf{b}-\mathbf{c}$	
{ [4] $P13$ (146, $R3$)	1; 7; 10	$\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}, \mathbf{a}-\mathbf{b}-\mathbf{c}$	
{ [4] $P13$ (146, $R3$)	1; 8; 11	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}, -\mathbf{a}-\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F23$ (196)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
{ $I2_13$ (199)	$\langle 5;\ 2+(0,1,0);\ 3+(1,0,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	
{ $I2_13$ (199)	$\langle 2+(2,1,0);\ 3+(3,0,0);\ 5+(1,-1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1,0,0$
{ $I2_13$ (199)	$\langle 2+(0,3,0);\ 3+(1,0,0);\ 5+(0,1,-1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0,1,0$
{ $I2_13$ (199)	$\langle 2+(0,1,0);\ 3+(1,0,2);\ 5+(-1,0,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0,0,1$
{ $I2_13$ (199)	$\langle 5;\ 2+(1,0,0);\ 3+(0,0,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2,1/2,1/2$
{ $I2_13$ (199)	$\langle 2+(3,0,0);\ 3+(2,0,1);\ 5+(1,-1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$3/2,1/2,1/2$
{ $I2_13$ (199)	$\langle 2+(1,2,0);\ 3+(0,0,1);\ 5+(0,1,-1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2,3/2,1/2$
{ $I2_13$ (199)	$\langle 2+(1,0,0);\ 3+(0,0,3);\ 5+(-1,0,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2,1/2,3/2$
{ $I23$ (197)	$\langle 2;\ 3;\ 5\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	
{ $I23$ (197)	$\langle (2;\ 3)+(2,0,0);\ 5+(1,-1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1,0,0$
{ $I23$ (197)	$\langle 3;\ 2+(0,2,0);\ 5+(0,1,-1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0,1,0$
{ $I23$ (197)	$\langle 2;\ 3+(0,0,2);\ 5+(-1,0,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$0,0,1$
{ $I23$ (197)	$\langle 5;\ 2+(1,1,0);\ 3+(1,0,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2,1/2,1/2$
{ $I23$ (197)	$\langle 2+(3,1,0);\ 3+(3,0,1);\ 5+(1,-1,0)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$3/2,1/2,1/2$
{ $I23$ (197)	$\langle 2+(1,3,0);\ 3+(1,0,1);\ 5+(0,1,-1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2,3/2,1/2$
{ $I23$ (197)	$\langle 2+(1,1,0);\ 3+(1,0,3);\ 5+(-1,0,1)\rangle$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$1/2,1/2,3/2$

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$			
$P23$ (195)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Pm\bar{3}$ (200); [2] $Pn\bar{3}$ (201); [2] $P432$ (207); [2] $P4_232$ (208); [2] $P\bar{4}3m$ (215); [2] $P\bar{4}3n$ (218)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I23$ (197); [4] $F23$ (196)

- **Decreased unit cell** none

T^2 $F23$ No. 196 $F23$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
48 *h* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
	(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$

I Maximal *translationengleiche* subgroups

[3] $F21$ (22, $F222$)	(1; 2; 3; 4)+	
[4] $F13$ (146, $R3$)	(1; 5; 9)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $F13$ (146, $R3$)	(1; 6; 12)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $F13$ (146, $R3$)	(1; 7; 10)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $F13$ (146, $R3$)	(1; 8; 11)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $P2_13$ (198)	1; 5; 9; (2; 7; 12) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 6; 11) + $(\frac{1}{2},0,\frac{1}{2})$	1/4, 1/4, 1/4
[4] $P2_13$ (198)	1; 7; 10; (2; 5; 11) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 8; 12) + $(\frac{1}{2},0,\frac{1}{2})$	3/4, 1/4, 3/4
[4] $P2_13$ (198)	1; 8; 11; (2; 6; 10) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 7; 9) + $(\frac{1}{2},0,\frac{1}{2})$	1/4, 3/4, 3/4
[4] $P2_13$ (198)	1; 6; 12; (2; 8; 9) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 5; 10) + $(\frac{1}{2},0,\frac{1}{2})$	3/4, 3/4, 1/4
[4] $P2_13$ (198)	1; 5; 9; (2; 7; 12) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 8; 10) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 6; 11) + $(\frac{1}{2},\frac{1}{2},0)$	
[4] $P2_13$ (198)	1; 7; 10; (2; 5; 11) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 6; 9) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 8; 12) + $(\frac{1}{2},\frac{1}{2},0)$	1/2, 1/2, 0
[4] $P2_13$ (198)	1; 8; 11; (2; 6; 10) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 5; 12) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 7; 9) + $(\frac{1}{2},\frac{1}{2},0)$	1/2, 0, 1/2
[4] $P2_13$ (198)	1; 6; 12; (2; 8; 9) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 7; 11) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 5; 10) + $(\frac{1}{2},\frac{1}{2},0)$	0, 1/2, 1/2
[4] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12	
[4] $P23$ (195)	1; 2; 3; 4; (5; 6; 7; 8) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12) + $(\frac{1}{2},\frac{1}{2},0)$	1/2, 0, 1/2
[4] $P23$ (195)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12) + $(0,\frac{1}{2},\frac{1}{2})$	1/2, 1/2, 0
[4] $P23$ (195)	1; 2; 3; 4; (5; 6; 7; 8) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12) + $(\frac{1}{2},0,\frac{1}{2})$	0, 1/2, 1/2
[4] $P23$ (195)	1; 5; 9; (2; 7; 12) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11) + $(0,\frac{1}{2},\frac{1}{2})$	1/4, 1/4, 1/4
[4] $P23$ (195)	1; 7; 10; (2; 5; 11) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12) + $(0,\frac{1}{2},\frac{1}{2})$	1/4, 3/4, 3/4
[4] $P23$ (195)	1; 8; 11; (2; 6; 10) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9) + $(0,\frac{1}{2},\frac{1}{2})$	3/4, 3/4, 1/4
[4] $P23$ (195)	1; 6; 12; (2; 8; 9) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10) + $(0,\frac{1}{2},\frac{1}{2})$	3/4, 1/4, 3/4

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$F23$ (196)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups

[2] $Fm\bar{3}$ (202); [2] $Fd\bar{3}$ (203); [2] $F432$ (209); [2] $F4_132$ (210); [2] $F\bar{4}3m$ (216); [2] $F\bar{4}3c$ (219)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{c}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P23$ (195)

$I23$ No. 197 $I23$ T^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
24 f 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
	(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$

I Maximal *translationengleiche* subgroups

[3] $I21$ (23, $I222$)	(1; 2; 3; 4)+	
[4] $I13$ (146, $R3$)	(1; 5; 9)+	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}, 1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$
[4] $I13$ (146, $R3$)	(1; 6; 12)+	$\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}, 1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$
[4] $I13$ (146, $R3$)	(1; 7; 10)+	$-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, 1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$
[4] $I13$ (146, $R3$)	(1; 8; 11)+	$\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}, 1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P23$ (195) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$I23$ (197)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Im\bar{3}$ (204); [2] $I432$ (211); [2] $I\bar{4}3m$ (217)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P23$ (195)

T^4 $P2_13$ No. 198 $P2_13$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
12	b	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[3] $P2_11$ (19, $P2_12_12_1$)	1; 2; 3; 4		
[4] $P13$ (146, $R3$)	1; 5; 9	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P13$ (146, $R3$)	1; 6; 12	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$0,1/2,1/2$
[4] $P13$ (146, $R3$)	1; 7; 10	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$1/2,1/2,0$
[4] $P13$ (146, $R3$)	1; 8; 11	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$1/2,0,1/2$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$P2_13$ (198)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2})$; $3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w)$; $5+(u-w,-u+v,-v+w)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Pa\bar{3}$ (205); [2] $P4_332$ (212); [2] $P4_132$ (213)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I2_13$ (199); [4] $F23$ (196)

- **Decreased unit cell** none

$I2_13$ No. 199 $I2_13$ T^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+\quad(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
24	c	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[3] $I2_11$ (24, $I2_12_12_1$)	(1; 2; 3; 4)+		
[4] $I13$ (146, $R3$)	(1; 5; 9)+	$-\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$	
[4] $I13$ (146, $R3$)	(1; 6; 12)+	$\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$	$0,1/2,1/2$
[4] $I13$ (146, $R3$)	(1; 7; 10)+	$-\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$	$1/2,1/2,0$
[4] $I13$ (146, $R3$)	(1; 8; 11)+	$\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$1/2,0,1/2$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P2_13$ (198) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$I2_13$ (199) $\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2});$ $3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w);$ $5+(u-w,-u+v,-v+w)\rangle$ $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ u,v,w

$p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$

p^3 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups

[2] $Ia\bar{3}$ (206); [2] $I4_132$ (214); [2] $I\bar{4}3d$ (220)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P23$ (195)

T_h^1 $\quad P2/m\bar{3}$ $\quad$ No. 200 $\quad Pm\bar{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

24	*l*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$	(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12	
[3] $Pm1$ (47, $Pmmm$)	1; 2; 3; 4; 13; 14; 15; 16	
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 5; 9; 13; 17; 21	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 8; 11; 13; 20; 23	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$Fm\bar{3}$ (202)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fm\bar{3}$ (202)	$\langle 2;\ 3;\ 5;\ 13+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$Ia\bar{3}$ (206)	$\langle 5;\ 13;\ 2+(0,1,0);\ 3+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Ia\bar{3}$ (206)	$\langle 2+(2,1,0);\ 3+(3,0,0);\ 5+(1,-1,0);\ 13+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$Ia\bar{3}$ (206)	$\langle 2+(0,3,0);\ 3+(1,0,0);\ 5+(0,1,-1);\ 13+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$Ia\bar{3}$ (206)	$\langle 2+(2,3,0);\ 3+(3,0,0);\ 5+(1,0,-1);\ 13+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,1,0$
$Ia\bar{3}$ (206)	$\langle 5;\ 13;\ 2+(1,0,0);\ 3+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$Ia\bar{3}$ (206)	$\langle 2+(3,0,0);\ 3+(2,0,1);\ 5+(1,-1,0);\ 13+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$Ia\bar{3}$ (206)	$\langle 2+(1,2,0);\ 3+(0,0,1);\ 5+(0,1,-1);\ 13+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$
$Ia\bar{3}$ (206)	$\langle 2+(3,2,0);\ 3+(2,0,1);\ 5+(1,0,-1);\ 13+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$
$Im\bar{3}$ (204)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Im\bar{3}$ (204)	$\langle (2;\ 3;\ 13)+(2,0,0);\ 5+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$Im\bar{3}$ (204)	$\langle 3;\ (2;\ 13)+(0,2,0);\ 5+(0,1,-1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$Im\bar{3}$ (204)	$\langle 2;\ (3;\ 13)+(0,0,2);\ 5+(-1,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,0,1$
$Im\bar{3}$ (204)	$\langle 5;\ 13;\ 2+(1,1,0);\ 3+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$Im\bar{3}$ (204)	$\langle 2+(3,1,0);\ 3+(2,1,0);\ 5+(1,-1,0);\ 13+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$Im\bar{3}$ (204)	$\langle 2+(1,3,0);\ 3+(0,1,0);\ 5+(0,1,-1);\ 13+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$
$Im\bar{3}$ (204)	$\langle 2+(3,3,0);\ 3+(2,1,0);\ 5+(1,0,-1);\ 13+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$			
$Pm\bar{3}$ (200)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);\ 5+(u-w,-u+v,-v+w);$ $13+(2u,2v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Pm\bar{3}m$ (221); [2] $Pm\bar{3}n$ (223)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

- **Decreased unit cell** none

$Pn\bar{3}$ No. 201 $P2/n\bar{3}$ T_h^2

ORIGIN CHOICE 1, Origin at 23, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre ($\bar{3}$)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
24	*h*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
			(17) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(19) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$
			(21) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(24) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[3] $Pn1$ (48, $Pnnn$)	1; 2; 3; 4; 13; 14; 15; 16		
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 5; 9; 13; 17; 21	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/4,1/4,1/4$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$3/4,1/4,3/4$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$1/4,3/4,3/4$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 8; 11; 13; 20; 23	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$3/4,3/4,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$Fd\bar{3}$ (203)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fd\bar{3}$ (203)	$\langle 2;\ 3;\ 5;\ 13+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$

- **Series of maximal isomorphic subgroups**

[p^3] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}$ (201)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2v);$ $5+(u-w,-u+v,-v+w);$ $13+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,\frac{p}{2}-\frac{1}{2}+2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

- **Decreased unit cell** none

ORIGIN CHOICE 2, Origin at centre $\bar{3}$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 23

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
24	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(15) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(16) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(19) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(20) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(23) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(24) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		1/4, 1/4, 1/4
[3] $Pn1$ (48, $Pnnn$)	1; 2; 3; 4; 13; 14; 15; 16		
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 5; 9; 13; 17; 21	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	1/2, 0, 1/2
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	0, 1/2, 1/2
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 8; 11; 13; 20; 23	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	1/2, 1/2, 0

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$Fd\bar{3}$ (203)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fd\bar{3}$ (203)	$\langle 2;\ 3;\ 5;\ 13+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 1/2, 1/2

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}$ (201) $\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0);$ $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ u,v,w
$3+(\frac{p}{2}-\frac{1}{2}+2u,0,\frac{p}{2}-\frac{1}{2}+2w);$
$5+(u-w,-u+v,-v+w);\ 13+(2u,2v,2w)\rangle$
$p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$
p^3 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups

[2] $Pn\bar{3}n$ (222); [2] $Pn\bar{3}m$ (224)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}$ (204); [4] $Fm\bar{3}$ (202)

- **Decreased unit cell** none

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 202, pp. 354–355.

$Fm\bar{3}$ No. 202 $F2/m\bar{3}$ T_h^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
96 i 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
	(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
	(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$
	(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$
	(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $F23$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+	
[3] $Fm1$ (69, $Fmmm$)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 5; 9; 13; 17; 21)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 6; 12; 13; 18; 24)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 7; 10; 13; 19; 22)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 8; 11; 13; 20; 23)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $Pa\bar{3}$ (205)	1; 5; 9; 13; 17; 21; (2; 7; 12; 14; 19; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 6; 11; 16; 18; 23) + $(\frac{1}{2},0,\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/2,1/2,0$
[4] $Pa\bar{3}$ (205)	1; 7; 10; 13; 19; 22; (2; 5; 11; 14; 17; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 8; 12; 16; 20; 24) + $(\frac{1}{2},0,\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$0,1/2,1/2$
[4] $Pa\bar{3}$ (205)	1; 8; 11; 13; 20; 23; (2; 6; 10; 14; 18; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 7; 9; 16; 19; 21) + $(\frac{1}{2},0,\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$1/2,0,1/2$
[4] $Pa\bar{3}$ (205)	1; 6; 12; 13; 18; 24; (2; 8; 9; 14; 20; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},\frac{1}{2},0)$; (4; 5; 10; 16; 17; 22) + $(\frac{1}{2},0,\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	
[4] $Pa\bar{3}$ (205)	1; 5; 9; 13; 17; 21; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 8; 10; 15; 20; 22) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(\frac{1}{2},\frac{1}{2},0)$		
[4] $Pa\bar{3}$ (205)	1; 7; 10; 13; 19; 22; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 6; 9; 15; 18; 21) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(\frac{1}{2},\frac{1}{2},0)$		$1/2,1/2,0$
[4] $Pa\bar{3}$ (205)	1; 8; 11; 13; 20; 23; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 5; 12; 15; 17; 24) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(\frac{1}{2},\frac{1}{2},0)$		$1/2,0,1/2$
[4] $Pa\bar{3}$ (205)	1; 6; 12; 13; 18; 24; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (3; 7; 11; 15; 19; 23) + $(0,\frac{1}{2},\frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(\frac{1}{2},\frac{1}{2},0)$		$0,1/2,1/2$

[4] $Pn\bar{3}$ (201)	1; 5; 9; 13; 17; 21; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(0,\frac{1}{2},\frac{1}{2})$		
[4] $Pn\bar{3}$ (201)	1; 7; 10; 13; 19; 22; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(0,\frac{1}{2},\frac{1}{2})$		$0,1/2,1/2$
[4] $Pn\bar{3}$ (201)	1; 8; 11; 13; 20; 23; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(0,\frac{1}{2},\frac{1}{2})$		$1/2,1/2,0$
[4] $Pn\bar{3}$ (201)	1; 6; 12; 13; 18; 24; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(0,\frac{1}{2},\frac{1}{2})$		$1/2,0,1/2$
[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		
[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},0)$		$1/2,0,1/2$
[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 21; 22; 23; 24) + $(0,\frac{1}{2},\frac{1}{2})$		$1/2,1/2,0$
[4] $Pm\bar{3}$ (200)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 17; 18; 19; 20) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$		$0,1/2,1/2$

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Fm\bar{3}$ (202)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);\ 5+(u-w,-u+v,-v+w);\ 13+(2u,2v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Fm\bar{3}m$ (225); [2] $Fm\bar{3}c$ (226)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pm\bar{3}$ (200)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 203, pp. 356–357.

$Fd\bar{3}$ No. 203 $F2/d\bar{3}$ T_h^4

ORIGIN CHOICE 1, Origin at 23, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre ($\bar{3}$)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+ \quad (\frac{1}{2},0,\frac{1}{2})+ \quad (\frac{1}{2},\frac{1}{2},0)+$

96	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(16) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$
			(17) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{z}+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$	(19) $z+\frac{1}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{1}{4}$
			(21) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{1}{4}$	(23) $\bar{y}+\frac{1}{4},z+\frac{1}{4},x+\frac{1}{4}$	(24) $y+\frac{1}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $F23$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		
[3] $Fd1$ (70, $Fddd$)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 5; 9; 13; 17; 21)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/8,1/8,1/8$
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 6; 12; 13; 18; 24)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$3/8,1/8,3/8$
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 7; 10; 13; 19; 22)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$	$1/8,3/8,3/8$
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 8; 11; 13; 20; 23)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$3/8,3/8,1/8$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell** none
- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Fd\bar{3}$ (203)	$\langle 2+(\frac{1}{2}+2u,\frac{1}{2}+2v,0);\ 3+(\frac{1}{2}+2u,0,\frac{1}{2}+2w);$ $5+(u-w,-u+v,-v+w);$ $13+(\frac{p}{4}+\frac{1}{4}+2u,\frac{p}{4}+\frac{1}{4}+2v,\frac{p}{4}+\frac{1}{4}+2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for prime $p\equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	$1/4+u,1/4+v,1/4+w$
$Fd\bar{3}$ (203)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);$ $13+(\frac{p}{4}-\frac{1}{4}+2u,\frac{p}{4}-\frac{1}{4}+2v,\frac{p}{4}-\frac{1}{4}+2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for prime $p\equiv 1$ (mod 4)	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Fd\bar{3}m$ (227); [2] $Fd\bar{3}c$ (228)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pn\bar{3}$ (201)

ORIGIN CHOICE 2, Origin at centre ($\bar{3}$), at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from 23

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+\quad(0,\frac{1}{2},\frac{1}{2})+\quad(\frac{1}{2},0,\frac{1}{2})+\quad(\frac{1}{2},\frac{1}{2},0)+$

96	g	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},z$	(3) $\bar{x}+\frac{3}{4},y,\bar{z}+\frac{3}{4}$	(4) $x,\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$
			(5) z,x,y	(6) $z,\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4},y$	(8) $\bar{z}+\frac{3}{4},x,\bar{y}+\frac{3}{4}$
			(9) y,z,x	(10) $\bar{y}+\frac{3}{4},z,\bar{x}+\frac{3}{4}$	(11) $y,\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4},x$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}$	(15) $x+\frac{1}{4},\bar{y},z+\frac{1}{4}$	(16) $\bar{x},y+\frac{1}{4},z+\frac{1}{4}$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x+\frac{1}{4},y+\frac{1}{4}$	(19) $z+\frac{1}{4},x+\frac{1}{4},\bar{y}$	(20) $z+\frac{1}{4},\bar{x},y+\frac{1}{4}$
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y+\frac{1}{4},\bar{z},x+\frac{1}{4}$	(23) $\bar{y},z+\frac{1}{4},x+\frac{1}{4}$	(24) $y+\frac{1}{4},z+\frac{1}{4},\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $F23$ (196)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		1/8, 1/8, 1/8
[3] $Fd1$ (70, $Fddd$)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 5; 9; 13; 17; 21)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 6; 12; 13; 18; 24)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$	1/4, 0, 1/4
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 7; 10; 13; 19; 22)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$	0, 1/4, 1/4
[4] $F1\bar{3}$ (148, $R\bar{3}$)	(1; 8; 11; 13; 20; 23)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$	1/4, 1/4, 0

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell** none
- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$Fd\bar{3}$ (203) $\langle 2+(\frac{3p}{4}-\frac{3}{4}+2u,\frac{3p}{4}-\frac{3}{4}+2v,0)$;
$3+(\frac{3p}{4}-\frac{3}{4}+2u,0,\frac{3p}{4}-\frac{3}{4}+2w)$;
$5+(u-w,-u+v,-v+w)$; $13+(2u,2v,2w)\rangle$
$p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$
p^3 conjugate subgroups for the prime p

$p\mathbf{a},p\mathbf{b},p\mathbf{c}$ $\quad u,v,w$

I Minimal *translationengleiche* supergroups

[2] $Fd\bar{3}m$ (227); [2] $Fd\bar{3}c$ (228)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pn\bar{3}$ (201)

$Im\bar{3}$ No. 204 $I2/m\bar{3}$ T_h^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

48	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $I23$ (197)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+	
[3] $Im1$ (71, $Immm$)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 5; 9; 13; 17; 21)+	$-\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 6; 12; 13; 18; 24)+	$\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 7; 10; 13; 19; 22)+	$-\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 8; 11; 13; 20; 23)+	$\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pn\bar{3}$ (201)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	1/4, 1/4, 1/4
[2] $Pm\bar{3}$ (200)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24	

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$Im\bar{3}$ (204)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);\ 5+(u-w,-u+v,-v+w);\ 13+(2u,2v,2w)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pm\bar{3}$ (200)

T_h^6 $\qquad P2_1/a\bar{3}$ $\qquad$ No. 205 $\qquad Pa\bar{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
24	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(15) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(19) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(20) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(24) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P2_13$ (198)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[3] $Pa1$ (61, $Pbca$)	1; 2; 3; 4; 13; 14; 15; 16		
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 5; 9; 13; 17; 21	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$0,1/2,1/2$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$1/2,1/2,0$
[4] $P1\bar{3}$ (148, $R\bar{3}$)	1; 8; 11; 13; 20; 23	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$1/2,0,1/2$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pa\bar{3}$ (205) $\quad \langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2});$
$3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w);$
$5+(u-w,-u+v,-v+w);\ 13+(2u,2v,2w)\rangle$
$p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$
p^3 conjugate subgroups for the prime p $\quad p\mathbf{a},p\mathbf{b},p\mathbf{c} \quad u,v,w$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Ia\bar{3}$ (206); [4] $Fm\bar{3}$ (202)

- **Decreased unit cell** none

$Ia\bar{3}$ No. 206 $I2_1/a\bar{3}$ T_h^7

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

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(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$
(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(15) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$
(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(19) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(20) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$
(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(24) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $I2_13$ (199)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		
[3] $Ia1$ (73, $Ibca$)	(1; 2; 3; 4; 13; 14; 15; 16)+		
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 5; 9; 13; 17; 21)+	$-\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$	
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 6; 12; 13; 18; 24)+	$\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$	$0,1/2,1/2$
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 7; 10; 13; 19; 22)+	$-\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$	$1/2,1/2,0$
[4] $I1\bar{3}$ (148, $R\bar{3}$)	(1; 8; 11; 13; 20; 23)+	$\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$1/2,0,1/2$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		
[2] $Pa\bar{3}$ (205)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$-\mathbf{b},\mathbf{a},\mathbf{c}$	$3/4,3/4,1/4$

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Ia\bar{3}$ (206)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2});\ 3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2u);$ $5+(u-w,-u+v,-v+w);\ 13+(2u,2v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Ia\bar{3}d$ (230)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pm\bar{3}$ (200)

O^1 $P432$ No. 207 $P432$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
24	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $P231$ (195, $P23$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12	
[3] $P412$ (89, $P422$)	1; 2; 3; 4; 13; 14; 15; 16	
[3] $P412$ (89, $P422$)	1; 4; 2; 3; 18; 19; 17; 20	$\mathbf{b},\mathbf{c},\mathbf{a}$
[3] $P412$ (89, $P422$)	1; 3; 4; 2; 22; 24; 23; 21	$\mathbf{c},\mathbf{a},\mathbf{b}$
[4] $P132$ (155, $R32$)	1; 5; 9; 14; 19; 24	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $P132$ (155, $R32$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $P132$ (155, $R32$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $P132$ (155, $R32$)	1; 8; 11; 14; 18; 22	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$F432$ (209)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$F432$ (209)	$\langle 2;\ 3;\ 5;\ 13+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$I432$ (211)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$I432$ (211)	$\langle 13;\ 2+(2,2,0);\ 3+(2,0,0);\ 5+(1,0,-1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,1,0$
$I432$ (211)	$\langle (2;\ 3)+(2,0,0);\ (5;\ 13)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$I432$ (211)	$\langle 3;\ 2+(0,2,0);\ 5+(0,1,-1);\ 13+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$I432$ (211)	$\langle 5;\ 2+(1,1,0);\ 3+(1,0,1);\ 13+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$I432$ (211)	$\langle 2+(3,3,0);\ 3+(3,0,1);\ 5+(1,0,-1);\ 13+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$
$I432$ (211)	$\langle 2+(3,1,0);\ 3+(3,0,1);\ 5+(1,-1,0);\ 13+(1,-1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$I432$ (211)	$\langle 2+(1,3,0);\ 3+(1,0,1);\ 5+(0,1,-1);\ 13+(-1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$

- **Series of maximal isomorphic subgroups**

[p^3] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$P432$ (207) $\langle 2+(2u,2v,0);\ 3+(2u,0,2w);\ 5+(u-w,-u+v,-v+w);$ $13+(u-v,-u+v,2w)\rangle$ $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ u,v,w

$p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$

p^3 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups

[2] $Pm\bar{3}m$ (221); [2] $Pn\bar{3}n$ (222)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I432$ (211); [4] $F432$ (209)

- **Decreased unit cell** none

$P4_232$ No. 208 $P4_232$ O^2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
24	*m*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P231$ (195, $P23$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[3] $P4_212$ (93, $P4_222$)	1; 2; 3; 4; 13; 14; 15; 16		$0,1/2,0$
[3] $P4_212$ (93, $P4_222$)	1; 4; 2; 3; 18; 19; 17; 20	$\mathbf{b},\mathbf{c},\mathbf{a}$	$0,0,1/2$
[3] $P4_212$ (93, $P4_222$)	1; 3; 4; 2; 22; 24; 23; 21	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/2,0,0$
[4] $P132$ (155, $R32$)	1; 5; 9; 14; 19; 24	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/4,1/4,1/4$
[4] $P132$ (155, $R32$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$-1/4,1/4,-1/4$
[4] $P132$ (155, $R32$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$1/4,-1/4,-1/4$
[4] $P132$ (155, $R32$)	1; 8; 11; 14; 18; 22	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$-1/4,-1/4,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$F4_132$ (210)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$F4_132$ (210)	$\langle 2;\ 3;\ 5;\ 13+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$			
$I4_132$ (214)	$\langle 5;\ 2+(0,1,0);\ (3;\ 13)+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$I4_132$ (214)	$\langle 2+(2,3,0);\ 3+(3,0,0);\ 5+(1,0,-1);$ $13+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,1,0$
$I4_132$ (214)	$\langle 2+(2,1,0);\ 3+(3,0,0);\ 5+(1,-1,0);$ $13+(2,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$I4_132$ (214)	$\langle 2+(0,3,0);\ 3+(1,0,0);\ 5+(0,1,-1);$ $13+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$I4_132$ (214)	$\langle 5;\ 2+(1,0,0);\ 3+(0,0,1);\ 13+(1,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$I4_132$ (214)	$\langle 2+(3,2,0);\ 3+(2,0,1);\ 5+(1,0,-1);$ $13+(1,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$
$I4_132$ (214)	$\langle 2+(3,0,0);\ 3+(2,0,1);\ 5+(1,-1,0);$ $13+(2,-1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$I4_132$ (214)	$\langle 2+(1,2,0);\ 3+(0,0,1);\ 5+(0,1,-1);$ $13+(0,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$			
$P4_232$ (208)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);$ $13+(\frac{p}{2}-\frac{1}{2}+u-v,\frac{p}{2}-\frac{1}{2}-u+v,\frac{p}{2}-\frac{1}{2}+2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Pm\bar{3}n$ (223); [2] $Pn\bar{3}m$ (224)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I432$ (211); [4] $F432$ (209)

- **Decreased unit cell** none

O^3 $F432$ No. 209 $F432$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

96	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $F231$ (196, $F23$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+	
[3] $F412$ (97, $I422$)	(1; 2; 3; 4; 13; 14; 15; 16)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$
[3] $F412$ (97, $I422$)	(1; 4; 2; 3; 18; 19; 17; 20)+	$1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c}), \mathbf{a}$
[3] $F412$ (97, $I422$)	(1; 3; 4; 2; 22; 24; 23; 21)+	$1/2(-\mathbf{a}+\mathbf{c}), 1/2(\mathbf{a}+\mathbf{c}), \mathbf{b}$
[4] $F132$ (155, $R32$)	(1; 5; 9; 14; 19; 24)+	$1/2(-\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}+\mathbf{c}), \mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $F132$ (155, $R32$)	(1; 6; 12; 13; 18; 24)+	$1/2(\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}-\mathbf{c}), -\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $F132$ (155, $R32$)	(1; 7; 10; 13; 19; 22)+	$1/2(-\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}-\mathbf{c}), \mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $F132$ (155, $R32$)	(1; 8; 11; 14; 18; 22)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}+\mathbf{c}), -\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $P4_232$ (208)	1; 5; 9; 14; 19; 24; (2; 7; 12; 13; 17; 21) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(0,\frac{1}{2},\frac{1}{2})$	1/4, 1/4, 1/4
[4] $P4_232$ (208)	1; 6; 12; 13; 18; 24; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11; 16; 17; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 15; 19; 23) + $(0,\frac{1}{2},\frac{1}{2})$	3/4, 1/4, 3/4
[4] $P4_232$ (208)	1; 7; 10; 13; 19; 22; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9; 16; 20; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 15; 18; 21) + $(0,\frac{1}{2},\frac{1}{2})$	1/4, 3/4, 3/4
[4] $P4_232$ (208)	1; 8; 11; 14; 18; 22; (2; 6; 10; 13; 20; 23) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(0,\frac{1}{2},\frac{1}{2})$	3/4, 3/4, 1/4
[4] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24	
[4] $P432$ (207)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$	1/2, 1/2, 0
[4] $P432$ (207)	1; 2; 3; 4; 17; 18; 19; 20; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$	0, 1/2, 1/2
[4] $P432$ (207)	1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$	1/2, 0, 1/2

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$F432$ (209)	$\langle 2+(2u,2v,0)$; $3+(2u,0,2w)$; $5+(u-w,-u+v,-v+w)$; $13+(u-v,-u+v,2w)\rangle$ $p>2$; $0 \le u < p$; $0 \le v < p$; $0 \le w < p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups

[2] $Fm\bar{3}m$ (225); [2] $Fm\bar{3}c$ (226)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P432$ (207)

$F4_132$ No. 210 $F4_132$ O^4

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

96	h	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $F231$ (196, $F23$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		
[3] $F4_112$ (98, $I4_122$)	(1; 2; 3; 4; 13; 14; 15; 16)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	
[3] $F4_112$ (98, $I4_122$)	(1; 4; 2; 3; 18; 19; 17; 20)+	$1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c}), \mathbf{a}$	
[3] $F4_112$ (98, $I4_122$)	(1; 3; 4; 2; 22; 24; 23; 21)+	$1/2(-\mathbf{a}+\mathbf{c}), 1/2(\mathbf{a}+\mathbf{c}), \mathbf{b}$	
[4] $F132$ (155, $R32$)	(1; 5; 9; 14; 19; 24)+	$1/2(-\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}+\mathbf{c}), \mathbf{a}+\mathbf{b}+\mathbf{c}$	1/8, 1/8, 1/8
[4] $F132$ (155, $R32$)	(1; 6; 12; 13; 18; 24)+	$1/2(\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}-\mathbf{c}), -\mathbf{a}+\mathbf{b}-\mathbf{c}$	3/8, 1/8, 3/8
[4] $F132$ (155, $R32$)	(1; 7; 10; 13; 19; 22)+	$1/2(-\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}-\mathbf{c}), \mathbf{a}-\mathbf{b}-\mathbf{c}$	1/8, 3/8, 3/8
[4] $F132$ (155, $R32$)	(1; 8; 11; 14; 18; 22)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}+\mathbf{c}), -\mathbf{a}-\mathbf{b}+\mathbf{c}$	3/8, 3/8, 1/8

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $P4_132$ (213)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24	1/4, 1/4, 1/4
[4] $P4_132$ (213)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$	3/4, 3/4, 1/4
[4] $P4_132$ (213)	1; 2; 3; 4; 17; 18; 19; 20; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$	1/4, 3/4, 3/4
[4] $P4_132$ (213)	1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$	3/4, 1/4, 3/4
[4] $P4_332$ (212)	1; 5; 9; 14; 19; 24; (2; 7; 12; 13; 17; 21) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10; 15; 20; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 16; 18; 23) + $(0,\frac{1}{2},\frac{1}{2})$	
[4] $P4_332$ (212)	1; 6; 12; 13; 18; 24; (2; 8; 9; 14; 20; 21) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11; 16; 17; 22) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 15; 19; 23) + $(0,\frac{1}{2},\frac{1}{2})$	1/2, 0, 1/2
[4] $P4_332$ (212)	1; 7; 10; 13; 19; 22; (2; 5; 11; 14; 17; 23) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9; 16; 20; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 15; 18; 21) + $(0,\frac{1}{2},\frac{1}{2})$	0, 1/2, 1/2
[4] $P4_332$ (212)	1; 8; 11; 14; 18; 22; (2; 6; 10; 13; 20; 23) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12; 15; 17; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 16; 19; 21) + $(0,\frac{1}{2},\frac{1}{2})$	1/2, 1/2, 0

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$F4_132$ (210)	$\langle 2+(\frac{1}{2}+2u,\frac{p}{2}+2v,\frac{p}{2}-\frac{1}{2})$; $3+(\frac{p}{2}+2u,\frac{p}{2}-\frac{1}{2},\frac{1}{2}+2w)$; $5+(u-w,-u+v,-v+w)$; $13+(\frac{3p}{4}-\frac{3}{4}+u-v,\frac{p}{4}-\frac{1}{4}-u+v,\frac{3p}{4}-\frac{1}{4}+2w)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for prime $p\equiv 3 \pmod 4$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	$1/4+u, 1/4+v, 1/4+w$
$F4_132$ (210)	$\langle 2+(2u,\frac{p}{2}-\frac{1}{2}+2v,\frac{p}{2}-\frac{1}{2})$; $3+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2},2w)$; $5+(u-w,-u+v,-v+w)$; $13+(\frac{3p}{4}-\frac{3}{4}+u-v,\frac{p}{4}-\frac{1}{4}-u+v,\frac{3p}{4}-\frac{3}{4}+2w)\rangle$ $p>4$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for prime $p\equiv 1 \pmod 4$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups

[2] $Fd\bar{3}m$ (227); [2] $Fd\bar{3}c$ (228)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P4_232$ (208)

$I432$ No. 211 $I432$ O^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

48	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$

I Maximal *translationengleiche* subgroups

[2] $I231$ (197, $I23$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+	
[3] $I412$ (97, $I422$)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[3] $I412$ (97, $I422$)	(1; 4; 2; 3; 18; 19; 17; 20)+	$\mathbf{b},\mathbf{c},\mathbf{a}$
[3] $I412$ (97, $I422$)	(1; 3; 4; 2; 22; 24; 23; 21)+	$\mathbf{c},\mathbf{a},\mathbf{b}$
[4] $I132$ (155, $R32$)	(1; 5; 9; 14; 19; 24)+	$-\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$
[4] $I132$ (155, $R32$)	(1; 6; 12; 13; 18; 24)+	$\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$
[4] $I132$ (155, $R32$)	(1; 7; 10; 13; 19; 22)+	$-\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$
[4] $I132$ (155, $R32$)	(1; 8; 11; 14; 18; 22)+	$\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = p\mathbf{c}$

$I432$ (211)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);$ $13+(u-v,-u+v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $P432$ (207)

O^6 $P4_332$ No. 212 $P4_332$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
24 *e* 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
	(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
	(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$
	(13) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{1}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{1}{4},z+\frac{3}{4}$
	(17) $x+\frac{1}{4},z+\frac{3}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{1}{4},y+\frac{3}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{3}{4},\bar{z}+\frac{3}{4},y+\frac{1}{4}$
	(21) $z+\frac{1}{4},y+\frac{3}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{3}{4},\bar{y}+\frac{3}{4},x+\frac{1}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{1}{4},x+\frac{3}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $P2_131$ (198, $P2_13$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[3] $P4_312$ (96, $P4_32_12$)	1; 2; 3; 4; 13; 14; 15; 16		$1/4,0,3/8$
[3] $P4_312$ (96, $P4_32_12$)	1; 4; 2; 3; 18; 19; 17; 20	$\mathbf{b},\mathbf{c},\mathbf{a}$	$3/8,1/4,0$
[3] $P4_312$ (96, $P4_32_12$)	1; 3; 4; 2; 22; 24; 23; 21	$\mathbf{c},\mathbf{a},\mathbf{b}$	$0,3/8,1/4$
[4] $P132$ (155, $R32$)	1; 5; 9; 14; 19; 24	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/8,1/8,1/8$
[4] $P132$ (155, $R32$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$7/8,5/8,3/8$
[4] $P132$ (155, $R32$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$5/8,3/8,7/8$
[4] $P132$ (155, $R32$)	1; 8; 11; 14; 18; 22	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$3/8,7/8,5/8$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$P4_132$ (213)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2})$; $3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w)$; $5+(u-w,-u+v,-v+w)$; $13+(\frac{3p}{4}-\frac{1}{4}+u-v,\frac{p}{4}-\frac{3}{4}-u+v,\frac{p}{4}-\frac{3}{4}+2w)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for prime $p\equiv 3$ (mod 4)	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w
$P4_332$ (212)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2})$; $3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w)$; $5+(u-w,-u+v,-v+w)$; $13+(\frac{p}{4}-\frac{1}{4}+u-v,\frac{3p}{4}-\frac{3}{4}-u+v,\frac{3p}{4}-\frac{3}{4}+2w)\rangle$ $p>4$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for prime $p\equiv 1$ (mod 4)	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4_132$ (214); [4] $F4_132$ (210)

- **Decreased unit cell** none

$P4_132$ No. 213 $P4_132$ O^7

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
24	*e*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $P2_131$ (198, $P2_13$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[3] $P4_112$ (92, $P4_12_12$)	1; 2; 3; 4; 13; 14; 15; 16		1/4, 1/2, 1/8
[3] $P4_112$ (92, $P4_12_12$)	1; 4; 2; 3; 18; 19; 17; 20	$\mathbf{b},\mathbf{c},\mathbf{a}$	1/8, 1/4, 1/2
[3] $P4_112$ (92, $P4_12_12$)	1; 3; 4; 2; 22; 24; 23; 21	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/2, 1/8, 1/4
[4] $P132$ (155, $R32$)	1; 5; 9; 14; 19; 24	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	3/8, 3/8, 3/8
[4] $P132$ (155, $R32$)	1; 6; 12; 13; 18; 24	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	5/8, 7/8, 1/8
[4] $P132$ (155, $R32$)	1; 7; 10; 13; 19; 22	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	7/8, 1/8, 5/8
[4] $P132$ (155, $R32$)	1; 8; 11; 14; 18; 22	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	1/8, 5/8, 7/8

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$P4_132$ (213) $\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2})$; $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ u,v,w
$3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w)$;
$5+(u-w,-u+v,-v+w)$;
$13+(\frac{3p}{4}-\frac{3}{4}+u-v,\frac{p}{4}-\frac{1}{4}-u+v,\frac{p}{4}-\frac{1}{4}+2w)\rangle$
$p>4$; $0\le u<p$; $0\le v<p$; $0\le w<p$
p^3 conjugate subgroups for prime $p\equiv 1$ (mod 4)

$P4_332$ (212) $\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2})$; $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ u,v,w
$3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w)$;
$5+(u-w,-u+v,-v+w)$;
$13+(\frac{p}{4}-\frac{3}{4}+u-v,\frac{3p}{4}-\frac{1}{4}-u+v,\frac{3p}{4}-\frac{1}{4}+2w)\rangle$
$p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$
p^3 conjugate subgroups for prime $p\equiv 3$ (mod 4)

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I4_132$ (214); [4] $F4_132$ (210)

- **Decreased unit cell** none

O^8 $I4_132$ No. 214 $I4_132$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

48	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $I2_131$ (199, $I2_13$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		
[3] $I4_112$ (98, $I4_122$)	(1; 2; 3; 4; 13; 14; 15; 16)+		0, 1/4, 1/8
[3] $I4_112$ (98, $I4_122$)	(1; 4; 2; 3; 18; 19; 17; 20)+	**b**, **c**, **a**	1/8, 0, 1/4
[3] $I4_112$ (98, $I4_122$)	(1; 3; 4; 2; 22; 24; 23; 21)+	**c**, **a**, **b**	1/4, 1/8, 0
[4] $I132$ (155, $R32$)	(1; 5; 9; 14; 19; 24)+	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}, 1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$	1/8, 1/8, 1/8
[4] $I132$ (155, $R32$)	(1; 6; 12; 13; 18; 24)+	$\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}, 1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$	7/8, 5/8, 3/8
[4] $I132$ (155, $R32$)	(1; 7; 10; 13; 19; 22)+	$-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, 1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$	5/8, 3/8, 7/8
[4] $I132$ (155, $R32$)	(1; 8; 11; 14; 18; 22)+	$\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}, 1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	3/8, 7/8, 5/8

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P4_132$ (213) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24

[2] $P4_332$ (212) 1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$I4_132$ (214) $\langle 2+(\frac{p}{2}-\frac{1}{2}+2u, 2v, \frac{p}{2}-\frac{1}{2})$; $3+(2u, \frac{p}{2}-\frac{1}{2}, \frac{p}{2}-\frac{1}{2}+2w)$; $5+(u-w, -u+v, -v+w)$; $13+(\frac{3p}{4}-\frac{3}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, \frac{p}{4}-\frac{1}{4}+2w)\rangle$ $\quad p\mathbf{a}, p\mathbf{b}, p\mathbf{c} \quad u,v,w$

$p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$

p^3 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups

[2] $Ia\bar{3}d$ (230)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P4_232$ (208)

$P\bar{4}3m$ No. 215 $P\bar{4}3m$ T_d^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
24	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$

I Maximal *translationengleiche* subgroups

[2] $P231$ (195, $P23$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12	
[3] $P\bar{4}1m$ (111, $P\bar{4}2m$)	1; 2; 3; 4; 13; 14; 15; 16	
[3] $P\bar{4}1m$ (111, $P\bar{4}2m$)	1; 4; 2; 3; 17; 20; 18; 19	$\mathbf{b},\mathbf{c},\mathbf{a}$
[3] $P\bar{4}1m$ (111, $P\bar{4}2m$)	1; 3; 4; 2; 21; 23; 24; 22	$\mathbf{c},\mathbf{a},\mathbf{b}$
[4] $P13m$ (160, $R3m$)	1; 5; 9; 13; 17; 21	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $P13m$ (160, $R3m$)	1; 6; 12; 14; 20; 21	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $P13m$ (160, $R3m$)	1; 7; 10; 14; 17; 23	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $P13m$ (160, $R3m$)	1; 8; 11; 13; 20; 23	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$F\bar{4}3c$ (219)	$\langle 2;\ 3;\ 5;\ 13+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$F\bar{4}3m$ (216)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$I\bar{4}3m$ (217)	$\langle 2;\ 3;\ 5;\ 13\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$I\bar{4}3m$ (217)	$\langle 13;\ 2+(2,2,0);\ 3+(2,0,0);\ 5+(1,0,-1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,1,0$
$I\bar{4}3m$ (217)	$\langle (2;\ 3)+(2,0,0);\ (5;\ 13)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$I\bar{4}3m$ (217)	$\langle 3;\ 2+(0,2,0);\ 5+(0,1,-1);\ 13+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$I\bar{4}3m$ (217)	$\langle 5;\ 13;\ 2+(1,1,0);\ 3+(1,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$I\bar{4}3m$ (217)	$\langle 13;\ 2+(3,3,0);\ 3+(3,0,1);\ 5+(1,0,-1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$
$I\bar{4}3m$ (217)	$\langle 2+(3,1,0);\ 3+(3,0,1);\ (5;\ 13)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$I\bar{4}3m$ (217)	$\langle 2+(1,3,0);\ 3+(1,0,1);\ 5+(0,1,-1);$ $13+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$P\bar{4}3m$ (215) $\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);\ 13+(u-v,-u+v,0)\rangle$ $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ u,v,w

$p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$

p^3 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups

[2] $Pm\bar{3}m$ (221); [2] $Pn\bar{3}m$ (224)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I\bar{4}3m$ (217); [4] $F\bar{4}3m$ (216)

- **Decreased unit cell** none

T_d^2 $F\bar{4}3m$ No. 216 $F\bar{4}3m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

96	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$	(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$

I Maximal *translationengleiche* subgroups

[2] $F231$ (196, $F23$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+	
[3] $F\bar{4}1m$ (119, $I\bar{4}m2$)	(1; 2; 3; 4; 13; 14; 15; 16)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$
[3] $F\bar{4}1m$ (119, $I\bar{4}m2$)	(1; 4; 2; 3; 17; 20; 18; 19)+	$1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c}),\mathbf{a}$
[3] $F\bar{4}1m$ (119, $I\bar{4}m2$)	(1; 3; 4; 2; 21; 23; 24; 22)+	$1/2(-\mathbf{a}+\mathbf{c}),1/2(\mathbf{a}+\mathbf{c}),\mathbf{b}$
[4] $F13m$ (160, $R3m$)	(1; 5; 9; 13; 17; 21)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $F13m$ (160, $R3m$)	(1; 6; 12; 14; 20; 21)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $F13m$ (160, $R3m$)	(1; 7; 10; 14; 17; 23)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $F13m$ (160, $R3m$)	(1; 8; 11; 13; 20; 23)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24	
[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$	$1/2,1/2,0$
[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 17; 18; 19; 20; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$	$0,1/2,1/2$
[4] $P\bar{4}3m$ (215)	1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$	$1/2,0,1/2$
[4] $P\bar{4}3m$ (215)	1; 5; 9; 13; 17; 21; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10; 16; 18; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 15; 20; 22) + $(0,\frac{1}{2},\frac{1}{2})$	$1/4,1/4,1/4$
[4] $P\bar{4}3m$ (215)	1; 6; 12; 14; 20; 21; (2; 8; 9; 13; 18; 24) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(0,\frac{1}{2},\frac{1}{2})$	$3/4,1/4,3/4$
[4] $P\bar{4}3m$ (215)	1; 7; 10; 14; 17; 23; (2; 5; 11; 13; 19; 22) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(0,\frac{1}{2},\frac{1}{2})$	$1/4,3/4,3/4$
[4] $P\bar{4}3m$ (215)	1; 8; 11; 13; 20; 23; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12; 16; 19; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 15; 17; 24) + $(0,\frac{1}{2},\frac{1}{2})$	$3/4,3/4,1/4$

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$F\bar{4}3m$ (216)	$\langle 2+(2u,2v,0)$; $3+(2u,0,2w)$; $5+(u-w,-u+v,-v+w)$; $13+(u-v,-u+v,0)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Fm\bar{3}m$ (225); [2] $Fd\bar{3}m$ (227)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}3m$ (215)

$I\bar{4}3m$ No. 217 $I\bar{4}3m$ T_d^3

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
48	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$

I Maximal *translationengleiche* subgroups

[2] $I231$ (197, $I23$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+	
[3] $I\bar{4}1m$ (121, $I\bar{4}2m$)	(1; 2; 3; 4; 13; 14; 15; 16)+	
[3] $I\bar{4}1m$ (121, $I\bar{4}2m$)	(1; 4; 2; 3; 17; 20; 18; 19)+	$\mathbf{b},\mathbf{c},\mathbf{a}$
[3] $I\bar{4}1m$ (121, $I\bar{4}2m$)	(1; 3; 4; 2; 21; 23; 24; 22)+	$\mathbf{c},\mathbf{a},\mathbf{b}$
[4] $I13m$ (160, $R3m$)	(1; 5; 9; 13; 17; 21)+	$-\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$
[4] $I13m$ (160, $R3m$)	(1; 6; 12; 14; 20; 21)+	$\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$
[4] $I13m$ (160, $R3m$)	(1; 7; 10; 14; 17; 23)+	$-\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$
[4] $I13m$ (160, $R3m$)	(1; 8; 11; 13; 20; 23)+	$\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24) + $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$I\bar{4}3m$ (217)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);\ 13+(u-v,-u+v,0)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Im\bar{3}m$ (229)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}3m$ (215)

T_d^4 $P\bar{4}3n$ No. 218 $P\bar{4}3n$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

24	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P231$ (195, $P23$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12		
[3] $P\bar{4}1n$ (112, $P\bar{4}2c$)	1; 2; 3; 4; 13; 14; 15; 16		$0,1/2,1/4$
[3] $P\bar{4}1n$ (112, $P\bar{4}2c$)	1; 4; 2; 3; 17; 20; 18; 19	$\mathbf{b},\mathbf{c},\mathbf{a}$	$1/4,0,1/2$
[3] $P\bar{4}1n$ (112, $P\bar{4}2c$)	1; 3; 4; 2; 21; 23; 24; 22	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/2,1/4,0$
[4] $P13n$ (161, $R3c$)	1; 5; 9; 13; 17; 21	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P13n$ (161, $R3c$)	1; 6; 12; 14; 20; 21	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	
[4] $P13n$ (161, $R3c$)	1; 7; 10; 14; 17; 23	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	
[4] $P13n$ (161, $R3c$)	1; 8; 11; 13; 20; 23	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$I\bar{4}3d$ (220)	$\langle 5;\ 13;\ 2+(0,1,0);\ 3+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$I\bar{4}3d$ (220)	$\langle 13;\ 2+(2,3,0);\ 3+(3,0,0);\ 5+(1,0,-1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,1,0$
$I\bar{4}3d$ (220)	$\langle 2+(2,1,0);\ 3+(3,0,0);\ (5;\ 13)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$I\bar{4}3d$ (220)	$\langle 2+(0,3,0);\ 3+(1,0,0);\ 5+(0,1,-1);\ 13+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$I\bar{4}3d$ (220)	$\langle 5;\ 13;\ 2+(1,0,0);\ 3+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$I\bar{4}3d$ (220)	$\langle 13;\ 2+(3,2,0);\ 3+(2,0,1);\ 5+(1,0,-1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$
$I\bar{4}3d$ (220)	$\langle 2+(3,0,0);\ 3+(2,0,1);\ (5;\ 13)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$I\bar{4}3d$ (220)	$\langle 2+(1,2,0);\ 3+(0,0,1);\ 5+(0,1,-1);\ 13+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$P\bar{4}3n$ (218) $\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$
$5+(u-w,-u+v,-v+w);$
$13+(\frac{p}{2}-\frac{1}{2}+u-v,\frac{p}{2}-\frac{1}{2}-u+v,\frac{p}{2}-\frac{1}{2})\rangle$
$p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$
p^3 conjugate subgroups for the prime p — $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ — u,v,w

I Minimal *translationengleiche* supergroups

[2] $Pn\bar{3}n$ (222); [2] $Pm\bar{3}n$ (223)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $I\bar{4}3m$ (217); [4] $F\bar{4}3c$ (219)

- **Decreased unit cell** none

$F\bar{4}3c$ No. 219 $F\bar{4}3c$ T_d^5

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

96	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $F231$ (196, $F23$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		
[3] $F\bar{4}1n$ (120, $I\bar{4}c2$)	(1; 2; 3; 4; 13; 14; 15; 16)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	$0,0,1/4$
[3] $F\bar{4}1n$ (120, $I\bar{4}c2$)	(1; 4; 2; 3; 17; 20; 18; 19)+	$1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c}),\mathbf{a}$	$1/4,0,0$
[3] $F\bar{4}1n$ (120, $I\bar{4}c2$)	(1; 3; 4; 2; 21; 23; 24; 22)+	$1/2(-\mathbf{a}+\mathbf{c}),1/2(\mathbf{a}+\mathbf{c}),\mathbf{b}$	$0,1/4,0$
[4] $F13n$ (161, $R3c$)	(1; 5; 9; 13; 17; 21)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $F13n$ (161, $R3c$)	(1; 6; 12; 14; 20; 21)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$	
[4] $F13n$ (161, $R3c$)	(1; 7; 10; 14; 17; 23)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$	
[4] $F13n$ (161, $R3c$)	(1; 8; 11; 13; 20; 23)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24	
[4] $P\bar{4}3n$ (218)	1; 2; 3; 4; 13; 14; 15; 16; (5; 6; 7; 8; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$	$1/2,1/2,0$
[4] $P\bar{4}3n$ (218)	1; 2; 3; 4; 17; 18; 19; 20; (5; 6; 7; 8; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24) + $(\frac{1}{2},0,\frac{1}{2})$	$0,1/2,1/2$
[4] $P\bar{4}3n$ (218)	1; 2; 3; 4; 21; 22; 23; 24; (5; 6; 7; 8; 17; 18; 19; 20) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16) + $(\frac{1}{2},\frac{1}{2},0)$	$1/2,0,1/2$
[4] $P\bar{4}3n$ (218)	1; 5; 9; 13; 17; 21; (2; 7; 12; 14; 19; 24) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10; 16; 18; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 15; 20; 22) + $(0,\frac{1}{2},\frac{1}{2})$	$1/4,1/4,1/4$
[4] $P\bar{4}3n$ (218)	1; 6; 12; 14; 20; 21; (2; 8; 9; 13; 18; 24) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11; 15; 19; 23) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 16; 17; 22) + $(0,\frac{1}{2},\frac{1}{2})$	$3/4,1/4,3/4$
[4] $P\bar{4}3n$ (218)	1; 7; 10; 14; 17; 23; (2; 5; 11; 13; 19; 22) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9; 15; 18; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 16; 20; 24) + $(0,\frac{1}{2},\frac{1}{2})$	$1/4,3/4,3/4$
[4] $P\bar{4}3n$ (218)	1; 8; 11; 13; 20; 23; (2; 6; 10; 14; 18; 22) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12; 16; 19; 21) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 15; 17; 24) + $(0,\frac{1}{2},\frac{1}{2})$	$3/4,3/4,1/4$

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$F\bar{4}3c$ (219)	$\langle 2+(2u,2v,0)$; $3+(2u,0,2w)$; $5+(u-w,-u+v,-v+w)$; $13+(\frac{p}{2}-\frac{1}{2}+u-v,\frac{p}{2}-\frac{1}{2}-u+v,\frac{p}{2}-\frac{1}{2})\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups

[2] $Fm\bar{3}c$ (226); [2] $Fd\bar{3}c$ (228)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}3m$ (215)

T_d^6 $\quad I\bar{4}3d$ $\quad$ No. 220 $\quad I\bar{4}3d$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

48	*e*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$
			(13) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(15) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$
			(17) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	(20) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$
			(21) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$	(22) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$

I Maximal *translationengleiche* subgroups

[2] $I2_13$1 (199, $I2_13$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12)+		
[3] $I\bar{4}1d$ (122, $I\bar{4}2d$)	(1; 2; 3; 4; 13; 14; 15; 16)+		1/2, 1/4, 1/8
[3] $I\bar{4}1d$ (122, $I\bar{4}2d$)	(1; 4; 2; 3; 17; 20; 18; 19)+	**b**, **c**, **a**	1/8, 1/2, 1/4
[3] $I\bar{4}1d$ (122, $I\bar{4}2d$)	(1; 3; 4; 2; 21; 23; 24; 22)+	**c**, **a**, **b**	1/4, 1/8, 1/2
[4] $I13d$ (161, $R3c$)	(1; 5; 9; 13; 17; 21)+	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}, 1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$	
[4] $I13d$ (161, $R3c$)	(1; 6; 12; 14; 20; 21)+	$\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}, 1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$	0, 1/2, 1/2
[4] $I13d$ (161, $R3c$)	(1; 7; 10; 14; 17; 23)+	$-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, 1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$	1/2, 1/2, 0
[4] $I13d$ (161, $R3c$)	(1; 8; 11; 13; 20; 23)+	$\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}, 1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	1/2, 0, 1/2

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell** none
- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$I\bar{4}3d$ (220) $\quad \langle 2+(\frac{p}{2}-\frac{1}{2}+2u, 2v, \frac{p}{2}-\frac{1}{2})$; $\quad p\mathbf{a}, p\mathbf{b}, p\mathbf{c} \quad u,v,w$
$3+(2u, \frac{p}{2}-\frac{1}{2}, \frac{p}{2}-\frac{1}{2}+2w)$;
$5+(u-w, -u+v, -v+w)$;
$13+(\frac{p}{4}-\frac{1}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, \frac{p}{4}-\frac{1}{4})\rangle$
$p>2$; $0 \le u < p$; $0 \le v < p$; $0 \le w < p$
p^3 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups

[2] $Ia\bar{3}d$ (230)

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a}$, $\mathbf{b}'=\frac{1}{2}\mathbf{b}$, $\mathbf{c}'=\frac{1}{2}\mathbf{c}$ $P\bar{4}3n$ (218)

$Pm\bar{3}m$ No. 221 $P4/m\bar{3}2/m$ O_h^1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

48	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$	(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$	(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48	
[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24	
[2] $Pm\bar{3}1$ (200, $Pm\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36	
[3] $P4/m12/m$ (123, $P4/mmm$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40	
[3] $P4/m12/m$ (123, $P4/mmm$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$
[3] $P4/m12/m$ (123, $P4/mmm$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$Fm\bar{3}m$ (225)	$\langle 2;\ 3;\ 5;\ 13;\ 25\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fm\bar{3}c$ (226)	$\langle 2;\ 3;\ 5;\ 25;\ 13+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fm\bar{3}c$ (226)	$\langle 2;\ 3;\ 5;\ 13;\ 25+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$Fm\bar{3}m$ (225)	$\langle 2;\ 3;\ 5;\ 13+(0,0,1);\ 25+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$Im\bar{3}m$ (229)	$\langle 2;\ 3;\ 5;\ 13;\ 25\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Im\bar{3}m$ (229)	$\langle 13;\ (2;\ 25)+(2,2,0);\ 3+(2,0,0);\ 5+(1,0,-1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,1,0$
$Im\bar{3}m$ (229)	$\langle (2;\ 3;\ 25)+(2,0,0);\ (5;\ 13)+(1,-1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$Im\bar{3}m$ (229)	$\langle 3;\ (2;\ 25)+(0,2,0);\ 5+(0,1,-1);\ 13+(-1,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$Im\bar{3}m$ (229)	$\langle 5;\ 25;\ (2;\ 13)+(0,0,1);\ 3+(0,1,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$Im\bar{3}m$ (229)	$\langle 2+(2,2,1);\ 3+(2,1,0);\ 5+(1,0,-1);\ 13+(0,0,1);\ 25+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$
$Im\bar{3}m$ (229)	$\langle 2+(2,0,1);\ 3+(2,1,0);\ 5+(1,-1,0);\ 13+(1,-1,1);\ 25+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$Im\bar{3}m$ (229)	$\langle 2+(0,2,1);\ 3+(0,1,0);\ 5+(0,1,-1);\ 13+(-1,1,1);\ 25+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pm\bar{3}m$ (221)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);\ 5+(u-w,-u+v,-v+w);$ $13+(u-v,-u+v,2w);\ 25+(2u,2v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

- **Decreased unit cell** none

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 222, pp. 377–378.

O_h^2 $P4/n\bar{3}2/n$ No. 222 $Pn\bar{3}n$

ORIGIN CHOICE 1, Origin at 432, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre ($\bar{3}$)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
48	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
			(25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
			(29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$
			(33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48		
[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		
[2] $Pn\bar{3}1$ (201, $Pn\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	$1/4,1/4,1/4$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$3/4,1/4,3/4$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$1/4,3/4,3/4$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$3/4,3/4,1/4$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}n$ (222)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);$ $13+(u-v,-u+v,2w);$ $25+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,\frac{p}{2}-\frac{1}{2}+2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

- **Decreased unit cell** none

$Pn\bar{3}n$ No. 222 $P4/n\bar{3}2/n$ O_h^2

ORIGIN CHOICE 2, Origin at centre ($\bar{3}$), at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 432

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

48	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$
			(13) $y,x,\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y,\bar{x}+\frac{1}{2},z$	(16) $\bar{y}+\frac{1}{2},x,z$
			(17) $x,z,\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z,y$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x,\bar{z}+\frac{1}{2},y$
			(21) $z,y,\bar{x}+\frac{1}{2}$	(22) $z,\bar{y}+\frac{1}{2},x$	(23) $\bar{z}+\frac{1}{2},y,x$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(27) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(28) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(32) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(35) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$
			(37) $\bar{y},\bar{x},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y},x+\frac{1}{2},\bar{z}$	(40) $y+\frac{1}{2},\bar{x},\bar{z}$
			(41) $\bar{x},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z},\bar{y}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x},z+\frac{1}{2},\bar{y}$
			(45) $\bar{z},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}$	(47) $z+\frac{1}{2},\bar{y},\bar{x}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48		$1/4,1/4,1/4$
[2] $P432$ (207)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		$1/4,1/4,1/4$
[2] $Pn\bar{3}1$ (201, $Pn\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40		
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[3] $P4/n12/n$ (126, $P4/nnc$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$1/2,0,1/2$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	$0,1/2,1/2$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$1/2,1/2,0$

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a}$, $\mathbf{b}'=p\mathbf{b}$, $\mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}n$ (222) $\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)$; $3+(\frac{p}{2}-\frac{1}{2}+2u,0,\frac{p}{2}-\frac{1}{2}+2w)$; $5+(u-w,-u+v,-v+w)$; $13+(u-v,-u+v,\frac{p}{2}-\frac{1}{2}+2w)$; $25+(2u,2v,2w)\rangle$ $p\mathbf{a},p\mathbf{b},p\mathbf{c}$ u,v,w

$p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$

p^3 conjugate subgroups for the prime p

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

- **Decreased unit cell** none

O_h^3 $\qquad$ $P4_2/m\bar{3}2/n$ $\qquad$ No. 223 $\qquad$ $Pm\bar{3}n$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

48 l 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$
(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$
(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$
(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$
(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$
(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3n$ (218)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48		
[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		
[2] $Pm\bar{3}1$ (200, $Pm\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36		
[3] $P4_2/m12/n$ (131, $P4_2/mmc$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40		$0,1/2,0$
[3] $P4_2/m12/n$ (131, $P4_2/mmc$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$	$0,0,1/2$
[3] $P4_2/m12/n$ (131, $P4_2/mmc$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$	$1/2,0,0$
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	
[4] $P1\bar{3}2/n$ (167, $R\bar{3}c$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[4] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$Ia\bar{3}d$ (230)	$\langle 5;\ 25;\ 2+(1,0,1);\ 3+(0,1,1);\ 13+(1,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Ia\bar{3}d$ (230)	$\langle 2+(3,2,1);\ 3+(2,1,1);\ 5+(1,0,-1);\ 13+(1,0,0);\ 25+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,1,0$
$Ia\bar{3}d$ (230)	$\langle 2+(3,0,1);\ 3+(2,1,1);\ 5+(1,-1,0);\ 13+(2,-1,0);\ 25+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1,0,0$
$Ia\bar{3}d$ (230)	$\langle 2+(1,2,1);\ 3+(0,1,1);\ 5+(0,1,-1);\ 13+(0,1,0);\ 25+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$0,1,0$
$Ia\bar{3}d$ (230)	$\langle 5;\ 25;\ 2+(0,1,1);\ 3+(1,1,0);\ 13+(1,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,1/2,1/2$
$Ia\bar{3}d$ (230)	$\langle 2+(2,3,1);\ 3+(3,1,0);\ 5+(1,0,-1);\ 13+(1,0,1);\ 25+(2,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,3/2,1/2$
$Ia\bar{3}d$ (230)	$\langle 2+(2,1,1);\ 3+(3,1,0);\ 5+(1,-1,0);\ 13+(2,-1,1);\ 25+(2,0,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$3/2,1/2,1/2$
$Ia\bar{3}d$ (230)	$\langle 2+(0,3,1);\ 3+(1,1,0);\ 5+(0,1,-1);\ 13+(0,1,1);\ 25+(0,2,0)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$1/2,3/2,1/2$

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pm\bar{3}n$ (223)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);\ 5+(u-w,-u+v,-v+w);$ $13+(\frac{p}{2}-\frac{1}{2}+u-v,\frac{p}{2}-\frac{1}{2}-u+v,\frac{p}{2}-\frac{1}{2}+2w);\ 25+(2u,2v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups $\qquad$ none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}c$ (226)

- **Decreased unit cell** $\qquad$ none

$Pn\bar{3}m$ No. 224 $P4_2/n\bar{3}2/m$ O_h^4

ORIGIN CHOICE 1, Origin at $\bar{4}3m$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre ($\bar{3}m$)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

48 l 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$
(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$
(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
(25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$
(29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$
(33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$
(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$
(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48		
[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		
[2] $Pn\bar{3}1$ (201, $Pn\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36		
[3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40		
[3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	1/4, 1/4, 1/4
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	3/4, 1/4, 3/4
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	1/4, 3/4, 3/4
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	3/4, 3/4, 1/4

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$Fd\bar{3}c$ (228)	$\langle 2;\ 3;\ 5;\ 25;\ 13+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 1/2, 1/2
$Fd\bar{3}c$ (228)	$\langle 2;\ 3;\ 5;\ 13;\ 25+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fd\bar{3}m$ (227)	$\langle 2;\ 3;\ 5;\ 13;\ 25\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fd\bar{3}m$ (227)	$\langle 2;\ 3;\ 5;\ (13;\ 25)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 1/2, 1/2

- **Series of maximal isomorphic subgroups**

[p^3] $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}m$ (224) $\quad \langle 2+(2u,2v,0);\ 3+(2u,0,2w);$
$5+(u-w,-u+v,-v+w);$
$13+(\frac{p}{2}-\frac{1}{2}+u-v,\frac{p}{2}-\frac{1}{2}-u+v,\frac{p}{2}-\frac{1}{2}+2w);$
$25+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,\frac{p}{2}-\frac{1}{2}+2w)\rangle$
$p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$
p^3 conjugate subgroups for the prime p $\quad p\mathbf{a},p\mathbf{b},p\mathbf{c} \quad u,v,w$

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

- **Decreased unit cell** none

(*Continued from the following page*)

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations**

[2] $Im\bar{3}m$ (229); [4] $Fm\bar{3}m$ (225)

- **Decreased unit cell** none

$Pn\bar{3}m$ No. 224 $P4_2/n\bar{3}2/m$ O_h^4

ORIGIN CHOICE 2, Origin at centre $(\bar{3}m)$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}3m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

48 l 1

(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$
(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$
(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$	(16) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$
(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}$	(18) $\bar{x},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{2},\bar{z},y+\frac{1}{2}$
(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}$	(22) $z+\frac{1}{2},\bar{y},x+\frac{1}{2}$	(23) $\bar{z},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z},\bar{y},\bar{x}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(27) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(28) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$
(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(32) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(35) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$
(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(38) y,x,z	(39) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	(40) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y$	(42) $x,\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) x,z,y	(44) $\bar{x}+\frac{1}{2},z,\bar{y}+\frac{1}{2}$
(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x$	(46) $\bar{z}+\frac{1}{2},y,\bar{x}+\frac{1}{2}$	(47) $z,\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3m$ (215)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48		1/4, 1/4, 1/4
[2] $P4_232$ (208)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24		1/4, 1/4, 1/4
[2] $Pn\bar{3}1$ (201, $Pn\bar{3}$)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36		
[3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40		0, 1/2, 0
[3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44	$\mathbf{b},\mathbf{c},\mathbf{a}$	0, 0, 1/2
[3] $P4_2/n12/m$ (134, $P4_2/nnm$)	1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45	$\mathbf{c},\mathbf{a},\mathbf{b}$	1/2, 0, 0
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48	$\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48	$-\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},-\mathbf{a}+\mathbf{b}-\mathbf{c}$	1/2, 0, 1/2
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46	$\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},\mathbf{a}-\mathbf{b}-\mathbf{c}$	0, 1/2, 1/2
[4] $P1\bar{3}2/m$ (166, $R\bar{3}m$)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46	$-\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},-\mathbf{a}-\mathbf{b}+\mathbf{c}$	1/2, 1/2, 0

II Maximal *klassengleiche* subgroups

- **Enlarged unit cell**

[2] $\mathbf{a}'=2\mathbf{a},\ \mathbf{b}'=2\mathbf{b},\ \mathbf{c}'=2\mathbf{c}$

$Fd\bar{3}c$ (228)	$\langle 2;\ 3;\ 5;\ 25;\ 13+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fd\bar{3}c$ (228)	$\langle 2;\ 3;\ 5;\ 13;\ 25+(1,1,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 1/2, 1/2
$Fd\bar{3}m$ (227)	$\langle 2;\ 3;\ 5;\ 13;\ 25\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	
$Fd\bar{3}m$ (227)	$\langle 2;\ 3;\ 5;\ (13;\ 25)+(0,0,1)\rangle$	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	1/2, 1/2, 1/2

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Pn\bar{3}m$ (224) $\quad p\mathbf{a},p\mathbf{b},p\mathbf{c} \quad u,v,w$

$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,\frac{p}{2}-\frac{1}{2}+2v,0)$;
$3+(\frac{p}{2}-\frac{1}{2}+2u,0,\frac{p}{2}-\frac{1}{2}+2w)$;
$5+(u-w,-u+v,-v+w)$;
$13+(\frac{p}{2}-\frac{1}{2}+u-v,\frac{p}{2}-\frac{1}{2}-u+v,2w)$;
$25+(2u,2v,2w)\rangle$
$p>2;\ 0\leq u<p;\ 0\leq v<p;\ 0\leq w<p$
p^3 conjugate subgroups for the prime p

(*Continued on the preceding page*)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 225, pp. 383–384.

O_h^5 $F\,4/m\,\bar{3}\,2/m$ No. 225 $F\,m\bar{3}m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

192 l 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
	(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
	(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
	(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$	(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
	(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$	(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
	(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+	
[2] $F432$ (209)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+	
[2] $Fm\bar{3}1$ (202, $Fm\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+	
[3] $F4/m12/m$ (139, $I4/mmm$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$
[3] $F4/m12/m$ (139, $I4/mmm$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c}),\mathbf{a}$
[3] $F4/m12/m$ (139, $I4/mmm$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$1/2(-\mathbf{a}+\mathbf{c}),1/2(\mathbf{a}+\mathbf{c}),\mathbf{b}$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $Pn\bar{3}m$ (224)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48; (2; 7; 12; 13; 17; 21; 26; 31; 36; 37; 41; 45) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10; 15; 20; 22; 27; 32; 34; 39; 44; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 16; 18; 23; 28; 30; 35; 40; 42; 47) + $(0,\frac{1}{2},\frac{1}{2})$	
[4] $Pn\bar{3}m$ (224)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48; (2; 8; 9; 14; 20; 21; 26; 32; 33; 38; 44; 45) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11; 16; 17; 22; 27; 31; 35; 40; 41; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 15; 19; 23; 28; 29; 34; 39; 43; 47) + $(0,\frac{1}{2},\frac{1}{2})$	$1/2,0,1/2$
[4] $Pn\bar{3}m$ (224)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46; (2; 5; 11; 14; 17; 23; 26; 29; 35; 38; 41; 47) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9; 16; 20; 24; 27; 30; 33; 40; 44; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 15; 18; 21; 28; 32; 36; 39; 42; 45) + $(0,\frac{1}{2},\frac{1}{2})$	$0,1/2,1/2$
[4] $Pn\bar{3}m$ (224)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46; (2; 6; 10; 13; 20; 23; 26; 30; 34; 37; 44; 47) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12; 15; 17; 24; 27; 29; 36; 39; 41; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 16; 19; 21; 28; 31; 33; 40; 43; 45) + $(0,\frac{1}{2},\frac{1}{2})$	$1/2,1/2,0$
[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48	
[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40; (5; 6; 7; 8; 21; 22; 23; 24; 29; 30; 31; 32; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 17; 18; 19; 20; 33; 34; 35; 36; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$	$1/2,1/2,0$
[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44; (5; 6; 7; 8; 13; 14; 15; 16; 29; 30; 31; 32; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24; 33; 34; 35; 36; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$	$0,1/2,1/2$
[4] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48; (5; 6; 7; 8; 17; 18; 19; 20; 29; 30; 31; 32; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16; 33; 34; 35; 36; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$	$1/2,0,1/2$

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = p\mathbf{c}$

$Fm\bar{3}m$ (225)	$\langle 2 + (2u, 2v, 0);\ 3 + (2u, 0, 2w);$ $5 + (u - w, -u + v, -v + w);$ $13 + (u - v, -u + v, 2w);\ 25 + (2u, 2v, 2w)\rangle$ $p > 2;\ 0 \le u < p;\ 0 \le v < p;\ 0 \le w < p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pm\bar{3}m$ (221)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 226, pp. 385–386.

O_h^6 $F4/m\bar{3}2/c$ No. 226 $Fm\bar{3}c$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

192 *j* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
	(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
	(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$
	(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$
	(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
	(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$
	(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
	(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$
	(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$
	(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$
	(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+		
[2] $F432$ (209)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+		1/4, 1/4, 1/4
[2] $Fm\bar{3}1$ (202, $Fm\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+		
[3] $F4_2/m12/n$ (140, $I4/mcm$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	1/4, 1/4, 0
[3] $F4_2/m12/n$ (140, $I4/mcm$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c}), \mathbf{a}$	0, 1/4, 1/4
[3] $F4_2/m12/n$ (140, $I4/mcm$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$1/2(-\mathbf{a}+\mathbf{c}), 1/2(\mathbf{a}+\mathbf{c}), \mathbf{b}$	1/4, 0, 1/4
[4] $F1\bar{3}2/n$ (167, $R\bar{3}c$)	(1; 5; 9; 25; 29; 33; 14; 19; 24; 38; 43; 48)+	$1/2(-\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}+\mathbf{c}), \mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $F1\bar{3}2/n$ (167, $R\bar{3}c$)	(1; 6; 12; 25; 30; 36; 13; 18; 24; 37; 42; 48)+	$1/2(\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}-\mathbf{c}), -\mathbf{a}+\mathbf{b}-\mathbf{c}$	
[4] $F1\bar{3}2/n$ (167, $R\bar{3}c$)	(1; 7; 10; 25; 31; 34; 13; 19; 22; 37; 43; 46)+	$1/2(-\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}-\mathbf{c}), \mathbf{a}-\mathbf{b}-\mathbf{c}$	
[4] $F1\bar{3}2/n$ (167, $R\bar{3}c$)	(1; 8; 11; 25; 32; 35; 14; 18; 22; 38; 42; 46)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}+\mathbf{c}), -\mathbf{a}-\mathbf{b}+\mathbf{c}$	

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48	
[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40; (5; 6; 7; 8; 21; 22; 23; 24; 29; 30; 31; 32; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (9; 10; 11; 12; 17; 18; 19; 20; 33; 34; 35; 36; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$	1/2, 1/2, 0
[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 17; 18; 19; 20; 25; 26; 27; 28; 41; 42; 43; 44; (5; 6; 7; 8; 13; 14; 15; 16; 29; 30; 31; 32; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$; (9; 10; 11; 12; 21; 22; 23; 24; 33; 34; 35; 36; 45; 46; 47; 48) + $(\frac{1}{2},0,\frac{1}{2})$	0, 1/2, 1/2
[4] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 21; 22; 23; 24; 25; 26; 27; 28; 45; 46; 47; 48; (5; 6; 7; 8; 17; 18; 19; 20; 29; 30; 31; 32; 41; 42; 43; 44) + $(0,\frac{1}{2},\frac{1}{2})$; (9; 10; 11; 12; 13; 14; 15; 16; 33; 34; 35; 36; 37; 38; 39; 40) + $(\frac{1}{2},\frac{1}{2},0)$	1/2, 0, 1/2

[4] $Pn\bar{3}n$ (222)	1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48; (2; 7; 12; 13; 17; 21; 26; 31; 36; 37; 41; 45) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 8; 10; 15; 20; 22; 27; 32; 34; 39; 44; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 6; 11; 16; 18; 23; 28; 30; 35; 40; 42; 47) + $(0,\frac{1}{2},\frac{1}{2})$		
[4] $Pn\bar{3}n$ (222)	1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48; (2; 8; 9; 14; 20; 21; 26; 32; 33; 38; 44; 45) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 7; 11; 16; 17; 22; 27; 31; 35; 40; 41; 46) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 5; 10; 15; 19; 23; 28; 29; 34; 39; 43; 47) + $(0,\frac{1}{2},\frac{1}{2})$		$1/2,0,1/2$
[4] $Pn\bar{3}n$ (222)	1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46; (2; 5; 11; 14; 17; 23; 26; 29; 35; 38; 41; 47) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 6; 9; 16; 20; 24; 27; 30; 33; 40; 44; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 8; 12; 15; 18; 21; 28; 32; 36; 39; 42; 45) + $(0,\frac{1}{2},\frac{1}{2})$		$0,1/2,1/2$
[4] $Pn\bar{3}n$ (222)	1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46; (2; 6; 10; 13; 20; 23; 26; 30; 34; 37; 44; 47) + $(\frac{1}{2},\frac{1}{2},0)$; (3; 5; 12; 15; 17; 24; 27; 29; 36; 39; 41; 48) + $(\frac{1}{2},0,\frac{1}{2})$; (4; 7; 9; 16; 19; 21; 28; 31; 33; 40; 43; 45) + $(0,\frac{1}{2},\frac{1}{2})$		$1/2,1/2,0$

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = p\mathbf{c}$

$Fm\bar{3}c$ (226)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);$ $5+(u-w,-u+v,-v+w);$ $13+(\frac{p}{2}-\frac{1}{2}+u-v,\frac{p}{2}-\frac{1}{2}-u+v,\frac{p}{2}-\frac{1}{2}+2w);$ $25+(2u,2v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pm\bar{3}m$ (221)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 227, pp. 387–389.

O_h^7 $\quad F\,4_1/d\,\bar{3}\,2/m$ $\quad$ No. 227 $\quad$ $F\,d\,\bar{3}\,m$

ORIGIN CHOICE 1, Origin at $\bar{4}3m$, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre ($\bar{3}m$)

Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+ \quad (\frac{1}{2},0,\frac{1}{2})+ \quad (\frac{1}{2},\frac{1}{2},0)+$

192 $\;i\;$ 1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
	(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$
	(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$
	(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$
	(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$
	(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$
	(25) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{3}{4}$	(27) $x+\frac{3}{4},\bar{y}+\frac{3}{4},z+\frac{1}{4}$	(28) $\bar{x}+\frac{3}{4},y+\frac{1}{4},z+\frac{3}{4}$
	(29) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(30) $\bar{z}+\frac{3}{4},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{3}{4}$	(32) $z+\frac{3}{4},\bar{x}+\frac{3}{4},y+\frac{1}{4}$
	(33) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	(34) $y+\frac{3}{4},\bar{z}+\frac{3}{4},x+\frac{1}{4}$	(35) $\bar{y}+\frac{3}{4},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{3}{4}$
	(37) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$
	(41) $\bar{x}+\frac{1}{2},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}$	(43) x,z,y	(44) $\bar{x},z+\frac{1}{2},\bar{y}+\frac{1}{2}$
	(45) $\bar{z}+\frac{1}{2},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}$	(48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+	
[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+	
[2] $Fd\bar{3}1$ (203, $Fd\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+	
[3] $F4_1/d12/m$ (141, $I4_1/amd$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$
[3] $F4_1/d12/m$ (141, $I4_1/amd$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c}),\mathbf{a}$
[3] $F4_1/d12/m$ (141, $I4_1/amd$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$1/2(-\mathbf{a}+\mathbf{c}),1/2(\mathbf{a}+\mathbf{c}),\mathbf{b}$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$ $1/8,1/8,1/8$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$ $3/8,1/8,3/8$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$ $1/8,3/8,3/8$
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$ $3/8,3/8,1/8$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** $\quad$ none
- **Enlarged unit cell** $\quad$ none

• **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = p\mathbf{c}$

$Fd\bar{3}m$ (227)	$\langle 2 + (\frac{1}{2} + 2u, \frac{p}{2} + 2v, \frac{p}{2} - \frac{1}{2});$ $3 + (\frac{p}{2} + 2u, \frac{p}{2} - \frac{1}{2}, \frac{1}{2} + 2w);$ $5 + (u - w, -u + v, -v + w);$ $13 + (\frac{3p}{4} - \frac{3}{4} + u - v, \frac{p}{4} - \frac{1}{4} - u + v, \frac{3p}{4} - \frac{1}{4} + 2w);$ $25 + (\frac{p}{4} + \frac{1}{4} + 2u, \frac{p}{4} + \frac{1}{4} + 2v, \frac{p}{4} + \frac{1}{4} + 2w)\rangle$ $p > 2;\ 0 \le u < p;\ 0 \le v < p;\ 0 \le w < p$ p^3 conjugate subgroups for prime $p \equiv 3 \pmod 4$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w
$Fd\bar{3}m$ (227)	$\langle 2 + (2u, \frac{p}{2} - \frac{1}{2} + 2v, \frac{p}{2} - \frac{1}{2});$ $3 + (\frac{p}{2} - \frac{1}{2} + 2u, \frac{p}{2} - \frac{1}{2}, 2w);$ $5 + (u - w, -u + v, -v + w);$ $13 + (\frac{3p}{4} - \frac{3}{4} + u - v, \frac{p}{4} - \frac{1}{4} - u + v, \frac{3p}{4} - \frac{3}{4} + 2w);$ $25 + (\frac{p}{4} - \frac{1}{4} + 2u, \frac{p}{4} - \frac{1}{4} + 2v, \frac{p}{4} - \frac{1}{4} + 2w)\rangle$ $p > 4;\ 0 \le u < p;\ 0 \le v < p;\ 0 \le w < p$ p^3 conjugate subgroups for prime $p \equiv 1 \pmod 4$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations** none

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)

$Fd\bar{3}m$ ORIGIN CHOICE 2 No. 227

(*Continued from the facing page*)

• **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = p\mathbf{c}$

$Fd\bar{3}m$ (227)	$\langle 2 + (\frac{3p}{4} - \frac{3}{4} + 2u, \frac{p}{4} - \frac{1}{4} + 2v, \frac{p}{2} - \frac{1}{2});$ $3 + (\frac{p}{4} - \frac{1}{4} + 2u, \frac{p}{2} - \frac{1}{2}, \frac{3p}{4} - \frac{3}{4} + 2w);$ $5 + (u - w, -u + v, -v + w);$ $13 + (\frac{3p}{4} - \frac{3}{4} + u - v, \frac{p}{4} - \frac{1}{4} - u + v, \frac{p}{2} - \frac{1}{2} + 2w);$ $25 + (2u, 2v, 2w)\rangle$ $p > 2;\ 0 \le u < p;\ 0 \le v < p;\ 0 \le w < p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

• **Additional centring translations** none

• **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)

ORIGIN CHOICE 2, Origin at centre $(\bar{3}m)$, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from $\bar{4}3m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

192 i 1

(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{4},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4}$
(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{y}+\frac{3}{4}$
(9) y,z,x	(10) $\bar{y}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$
(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$
(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{2},y+\frac{3}{4}$
(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{2},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{2},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z},\bar{y},\bar{x}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{3}{4},\bar{y}+\frac{1}{2},z+\frac{1}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{4},z+\frac{3}{4}$
(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{3}{4},\bar{x}+\frac{1}{2},y+\frac{1}{4}$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{3}{4},\bar{z}+\frac{1}{2},x+\frac{1}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{1}{2}$
(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y}+\frac{3}{4},x+\frac{1}{2},\bar{z}+\frac{1}{4}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$
(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) x,z,y	(44) $\bar{x}+\frac{3}{4},z+\frac{1}{2},\bar{y}+\frac{1}{4}$
(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{1}{2}$	(46) $\bar{z}+\frac{3}{4},y+\frac{1}{2},\bar{x}+\frac{1}{4}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3m$ (216)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+		1/8, 1/8, 1/8
[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+		3/8, 3/8, 3/8
[2] $Fd\bar{3}1$ (203, $Fd\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+		
[3] $F4_1/d12/m$ (141, $I4_1/amd$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	1/4, 1/4, 0
[3] $F4_1/d12/m$ (141, $I4_1/amd$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c}), \mathbf{a}$	0, 1/4, 1/4
[3] $F4_1/d12/m$ (141, $I4_1/amd$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$1/2(-\mathbf{a}+\mathbf{c}), 1/2(\mathbf{a}+\mathbf{c}), \mathbf{b}$	1/4, 0, 1/4
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+	$1/2(-\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}+\mathbf{c}), \mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+	$1/2(\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}-\mathbf{c}), -\mathbf{a}+\mathbf{b}-\mathbf{c}$	1/4, 0, 1/4
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+	$1/2(-\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}-\mathbf{c}), \mathbf{a}-\mathbf{b}-\mathbf{c}$	0, 1/4, 1/4
[4] $F1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}+\mathbf{c}), -\mathbf{a}-\mathbf{b}+\mathbf{c}$	1/4, 1/4, 0

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell** none

(*Continued on the facing page*)

International Tables for Crystallography (2006). Vol. A1, Maximal subgroups of space group 228, pp. 390–392.

$F d\bar{3}c$ No. 228 $F4_1/d\bar{3}2/c$ O_h^8

ORIGIN CHOICE 1, Origin at 23, at $-\frac{3}{8},-\frac{3}{8},-\frac{3}{8}$ from centre ($\bar{3}$)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity, Wyckoff letter, Site symmetry — Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

192	h	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$
			(25) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(26) $x+\frac{3}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(27) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{3}{4}$	(28) $\bar{x}+\frac{1}{4},y+\frac{3}{4},z+\frac{1}{4}$
			(29) $\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(30) $\bar{z}+\frac{1}{4},x+\frac{3}{4},y+\frac{1}{4}$	(31) $z+\frac{3}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$	(32) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{3}{4}$
			(33) $\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4}$	(34) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{3}{4}$	(35) $\bar{y}+\frac{1}{4},z+\frac{3}{4},x+\frac{1}{4}$	(36) $y+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$
			(37) $\bar{y},\bar{x}+\frac{1}{2},z$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x,\bar{z}$	(40) $y,\bar{x},\bar{z}+\frac{1}{2}$
			(41) $\bar{x},\bar{z}+\frac{1}{2},y$	(42) $x,\bar{z},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z,\bar{y}$
			(45) $\bar{z},\bar{y}+\frac{1}{2},x$	(46) $\bar{z}+\frac{1}{2},y,\bar{x}$	(47) $z,\bar{y},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+		
[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+		
[2] $Fd\bar{3}1$ (203, $Fd\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+		1/4, 1/4, 1/4
[3] $F4_1/d12/c$ (142, $I4_1/acd$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{a}+\mathbf{b}), \mathbf{c}$	0, 0, 1/4
[3] $F4_1/d12/c$ (142, $I4_1/acd$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$1/2(\mathbf{b}-\mathbf{c}), 1/2(\mathbf{b}+\mathbf{c}), \mathbf{a}$	1/4, 0, 0
[3] $F4_1/d12/c$ (142, $I4_1/acd$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$1/2(-\mathbf{a}+\mathbf{c}), 1/2(\mathbf{a}+\mathbf{c}), \mathbf{b}$	0, 1/4, 0
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+	$1/2(-\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}+\mathbf{c}), \mathbf{a}+\mathbf{b}+\mathbf{c}$	3/8, 3/8, 3/8
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+	$1/2(\mathbf{a}+\mathbf{b}), 1/2(-\mathbf{b}-\mathbf{c}), -\mathbf{a}+\mathbf{b}-\mathbf{c}$	1/8, 3/8, 1/8
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+	$1/2(-\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}-\mathbf{c}), \mathbf{a}-\mathbf{b}-\mathbf{c}$	3/8, 1/8, 1/8
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+	$1/2(\mathbf{a}-\mathbf{b}), 1/2(\mathbf{b}+\mathbf{c}), -\mathbf{a}-\mathbf{b}+\mathbf{c}$	1/8, 1/8, 3/8

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$Fd\bar{3}c$ (228)	$\langle 2+(\frac{1}{2}+2u, \frac{p}{2}+2v, \frac{p}{2}-\frac{1}{2});\ 3+(\frac{p}{2}+2u, \frac{p}{2}-\frac{1}{2}, \frac{1}{2}+2w);$ $5+(u-w, -u+v, -v+w);$ $13+(\frac{3p}{4}-\frac{3}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, \frac{3p}{4}-\frac{1}{4}+2w);$ $25+(\frac{3p}{4}-\frac{1}{4}+2u, \frac{3p}{4}-\frac{1}{4}+2v, \frac{3p}{4}-\frac{1}{4}+2w)\rangle$ $p>2;\ 0 \le u < p;\ 0 \le v < p;\ 0 \le w < p$ p^3 conjugate subgroups for prime $p \equiv 3 \pmod 4$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	$1/4+u, 1/4+v, 1/4+w$
$Fd\bar{3}c$ (228)	$\langle 2+(2u, \frac{p}{2}-\frac{1}{2}+2v, \frac{p}{2}-\frac{1}{2});\ 3+(\frac{p}{2}-\frac{1}{2}+2u, \frac{p}{2}-\frac{1}{2}, 2w);$ $5+(u-w, -u+v, -v+w);$ $13+(\frac{3p}{4}-\frac{3}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, \frac{3p}{4}-\frac{3}{4}+2w);$ $25+(\frac{3p}{4}-\frac{3}{4}+2u, \frac{3p}{4}-\frac{3}{4}+2v, \frac{3p}{4}-\frac{3}{4}+2w)\rangle$ $p>4;\ 0 \le u < p;\ 0 \le v < p;\ 0 \le w < p$ p^3 conjugate subgroups for prime $p \equiv 1 \pmod 4$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$

$Fd\bar{3}c$ (228)	$\langle 2+(\frac{p}{4}-\frac{1}{4}+2u, \frac{3p}{4}-\frac{3}{4}+2v, \frac{p}{2}-\frac{1}{2});$ $3+(\frac{3p}{4}-\frac{3}{4}+2u, \frac{p}{2}-\frac{1}{2}, \frac{p}{4}-\frac{1}{4}+2w);$ $5+(u-w, -u+v, -v+w);$ $13+(\frac{3p}{4}-\frac{3}{4}+u-v, \frac{p}{4}-\frac{1}{4}-u+v, 2w);\ 25+(2u, 2v, 2w)\rangle$ $p>2;\ 0 \le u < p;\ 0 \le v < p;\ 0 \le w < p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	u, v, w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[2] $\mathbf{a}' = \frac{1}{2}\mathbf{a}$, $\mathbf{b}' = \frac{1}{2}\mathbf{b}$, $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pn\bar{3}m$ (224)

$F\,d\,\bar{3}\,c$ No. 228 $F\,4_1/d\,\bar{3}\,2/c$ O_h^8

ORIGIN CHOICE 2, Origin at centre ($\bar{3}$), at $\frac{3}{8},\frac{3}{8},\frac{3}{8}$ from 23

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+\quad (0,\frac{1}{2},\frac{1}{2})+\quad (\frac{1}{2},0,\frac{1}{2})+\quad (\frac{1}{2},\frac{1}{2},0)+$

192 h 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{4},\bar{y}+\frac{3}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{3}{4},y+\frac{1}{2},\bar{z}+\frac{1}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{z}+\frac{3}{4}$
	(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(7) $\bar{z}+\frac{1}{4},\bar{x}+\frac{3}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{3}{4},x+\frac{1}{2},\bar{y}+\frac{1}{4}$
	(9) y,z,x	(10) $\bar{y}+\frac{3}{4},z+\frac{1}{2},\bar{x}+\frac{1}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(12) $\bar{y}+\frac{1}{4},\bar{z}+\frac{3}{4},x+\frac{1}{2}$
	(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{4},\bar{x},z+\frac{3}{4}$	(16) $\bar{y},x+\frac{3}{4},z+\frac{1}{4}$
	(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}$	(18) $\bar{x},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{4},\bar{z},y+\frac{3}{4}$
	(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}$	(22) $z+\frac{1}{4},\bar{y},x+\frac{3}{4}$	(23) $\bar{z},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$
	(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{3}{4},y+\frac{1}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{4},\bar{y}+\frac{1}{2},z+\frac{3}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{3}{4},z+\frac{1}{4}$
	(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{3}{4},y+\frac{1}{4}$	(31) $z+\frac{3}{4},x+\frac{1}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{4},\bar{x}+\frac{1}{2},y+\frac{3}{4}$
	(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$	(36) $y+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$
	(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{3}{4},x,\bar{z}+\frac{1}{4}$	(40) $y,\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$
	(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y$	(42) $x,\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{3}{4},z,\bar{y}+\frac{1}{4}$
	(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x$	(46) $\bar{z}+\frac{3}{4},y,\bar{x}+\frac{1}{4}$	(47) $z,\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$

I Maximal *translationengleiche* subgroups

[2] $F\bar{4}3c$ (219)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+		$1/8,1/8,1/8$
[2] $F4_132$ (210)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+		$1/8,1/8,1/8$
[2] $Fd\bar{3}1$ (203, $Fd\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+		
[3] $F4_1/d12/c$ (142, $I4_1/acd$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{a}+\mathbf{b}),\mathbf{c}$	
[3] $F4_1/d12/c$ (142, $I4_1/acd$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$1/2(\mathbf{b}-\mathbf{c}),1/2(\mathbf{b}+\mathbf{c}),\mathbf{a}$	
[3] $F4_1/d12/c$ (142, $I4_1/acd$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$1/2(-\mathbf{a}+\mathbf{c}),1/2(\mathbf{a}+\mathbf{c}),\mathbf{b}$	
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+	$1/2(-\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}+\mathbf{c}),\mathbf{a}+\mathbf{b}+\mathbf{c}$	
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+	$1/2(\mathbf{a}+\mathbf{b}),1/2(-\mathbf{b}-\mathbf{c}),-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$1/4,0,1/4$
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+	$1/2(-\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}-\mathbf{c}),\mathbf{a}-\mathbf{b}-\mathbf{c}$	$0,1/4,1/4$
[4] $F1\bar{3}2/c$ (167, $R\bar{3}c$)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+	$1/2(\mathbf{a}-\mathbf{b}),1/2(\mathbf{b}+\mathbf{c}),-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$1/4,1/4,0$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell** none

(*Continued on the preceding page*)

O_h^9 $\quad I4/m\bar{3}2/m$ $\quad$ No. 229 $\quad Im\bar{3}m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

96 *l* 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$	(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$	(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}3m$ (217)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+	
[2] $I432$ (211)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+	
[2] $Im\bar{3}1$ (204, $Im\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+	
{ [3] $I4/m12/m$ (139, $I4/mmm$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+	
{ [3] $I4/m12/m$ (139, $I4/mmm$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$\mathbf{b},\mathbf{c},\mathbf{a}$
{ [3] $I4/m12/m$ (139, $I4/mmm$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$\mathbf{c},\mathbf{a},\mathbf{b}$
{ [4] $I1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+	$-\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$
{ [4] $I1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+	$\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$
{ [4] $I1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+	$-\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$
{ [4] $I1\bar{3}2/m$ (166, $R\bar{3}m$)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+	$\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations**

[2] $Pn\bar{3}m$ (224)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36) $+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$1/4,1/4,1/4$
[2] $Pm\bar{3}n$ (223)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; (13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) $+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})$	
[2] $Pn\bar{3}n$ (222)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; (25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48) $+ (\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$1/4,1/4,1/4$
[2] $Pm\bar{3}m$ (221)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48	

- **Enlarged unit cell** none

- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}' = p\mathbf{a},\ \mathbf{b}' = p\mathbf{b},\ \mathbf{c}' = p\mathbf{c}$

$Im\bar{3}m$ (229)	$\langle 2+(2u,2v,0);\ 3+(2u,0,2w);\ 5+(u-w,-u+v,-v+w);\ 13+(u-v,-u+v,2w);\ 25+(2u,2v,2w)\rangle$ $p>2;\ 0\le u<p;\ 0\le v<p;\ 0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none

- **Decreased unit cell**

[4] $\mathbf{a}' = \frac{1}{2}\mathbf{a},\ \mathbf{b}' = \frac{1}{2}\mathbf{b},\ \mathbf{c}' = \frac{1}{2}\mathbf{c}$ $Pm\bar{3}m$ (221)

$Ia\bar{3}d$ No. 230 $I4_1/a\bar{3}2/d$ O_h^{10}

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

General position

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

96	*h*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(27) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(31) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(32) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(36) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(38) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	(39) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	(40) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	(42) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$	(44) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(46) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$	(47) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$

I Maximal *translationengleiche* subgroups

[2] $I\bar{4}3d$ (220)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 37; 38; 39; 40; 41; 42; 43; 44; 45; 46; 47; 48)+		
[2] $I4_132$ (214)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 18; 19; 20; 21; 22; 23; 24)+		
[2] $Ia\bar{3}1$ (206, $Ia\bar{3}$)	(1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12; 25; 26; 27; 28; 29; 30; 31; 32; 33; 34; 35; 36)+		
[3] $I4_1/a12/d$ (142, $I4_1/acd$)	(1; 2; 3; 4; 13; 14; 15; 16; 25; 26; 27; 28; 37; 38; 39; 40)+		
[3] $I4_1/a12/d$ (142, $I4_1/acd$)	(1; 4; 2; 3; 18; 19; 17; 20; 25; 28; 26; 27; 42; 43; 41; 44)+	$\mathbf{b},\mathbf{c},\mathbf{a}$	
[3] $I4_1/a12/d$ (142, $I4_1/acd$)	(1; 3; 4; 2; 22; 24; 23; 21; 25; 27; 28; 26; 46; 48; 47; 45)+	$\mathbf{c},\mathbf{a},\mathbf{b}$	
[4] $I1\bar{3}2/d$ (167, $R\bar{3}c$)	(1; 5; 9; 14; 19; 24; 25; 29; 33; 38; 43; 48)+	$-\mathbf{a}+\mathbf{b},-\mathbf{b}+\mathbf{c},1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$	
[4] $I1\bar{3}2/d$ (167, $R\bar{3}c$)	(1; 6; 12; 13; 18; 24; 25; 30; 36; 37; 42; 48)+	$\mathbf{a}+\mathbf{b},-\mathbf{b}-\mathbf{c},1/2(-\mathbf{a}+\mathbf{b}-\mathbf{c})$	$0,1/2,1/2$
[4] $I1\bar{3}2/d$ (167, $R\bar{3}c$)	(1; 7; 10; 13; 19; 22; 25; 31; 34; 37; 43; 46)+	$-\mathbf{a}-\mathbf{b},\mathbf{b}-\mathbf{c},1/2(\mathbf{a}-\mathbf{b}-\mathbf{c})$	$1/2,1/2,0$
[4] $I1\bar{3}2/d$ (167, $R\bar{3}c$)	(1; 8; 11; 14; 18; 22; 25; 32; 35; 38; 42; 46)+	$\mathbf{a}-\mathbf{b},\mathbf{b}+\mathbf{c},1/2(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$1/2,0,1/2$

II Maximal *klassengleiche* subgroups

- **Loss of centring translations** none
- **Enlarged unit cell** none
- **Series of maximal isomorphic subgroups**

$[p^3]$ $\mathbf{a}'=p\mathbf{a},\ \mathbf{b}'=p\mathbf{b},\ \mathbf{c}'=p\mathbf{c}$

$Ia\bar{3}d$ (230)	$\langle 2+(\frac{p}{2}-\frac{1}{2}+2u,2v,\frac{p}{2}-\frac{1}{2})$; $3+(2u,\frac{p}{2}-\frac{1}{2},\frac{p}{2}-\frac{1}{2}+2w)$; $5+(u-w,-u+v,-v+w)$; $13+(\frac{3p}{4}-\frac{3}{4}+u-v,\frac{p}{4}-\frac{1}{4}-u+v,\frac{p}{4}-\frac{1}{4}+2w)$; $25+(2u,2v,2w)\rangle$ $p>2$; $0\le u<p$; $0\le v<p$; $0\le w<p$ p^3 conjugate subgroups for the prime p	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	u,v,w

I Minimal *translationengleiche* supergroups none

II Minimal non-isomorphic *klassengleiche* supergroups

- **Additional centring translations** none
- **Decreased unit cell**

[4] $\mathbf{a}'=\frac{1}{2}\mathbf{a},\ \mathbf{b}'=\frac{1}{2}\mathbf{b},\ \mathbf{c}'=\frac{1}{2}\mathbf{c}$ $Pm\bar{3}n$ (223)

International Tables for Crystallography (2006). Vol. A1, Chapter 2.4, pp. 395–414.

2.4. Graphs for *translationengleiche* subgroups

BY VOLKER GRAMLICH AND HANS WONDRATSCHEK

2.4.1. Graphs of the *translationengleiche* subgroups with a cubic summit

For an explanation of these graphs, see Section 2.1.7.2 (p. 54).

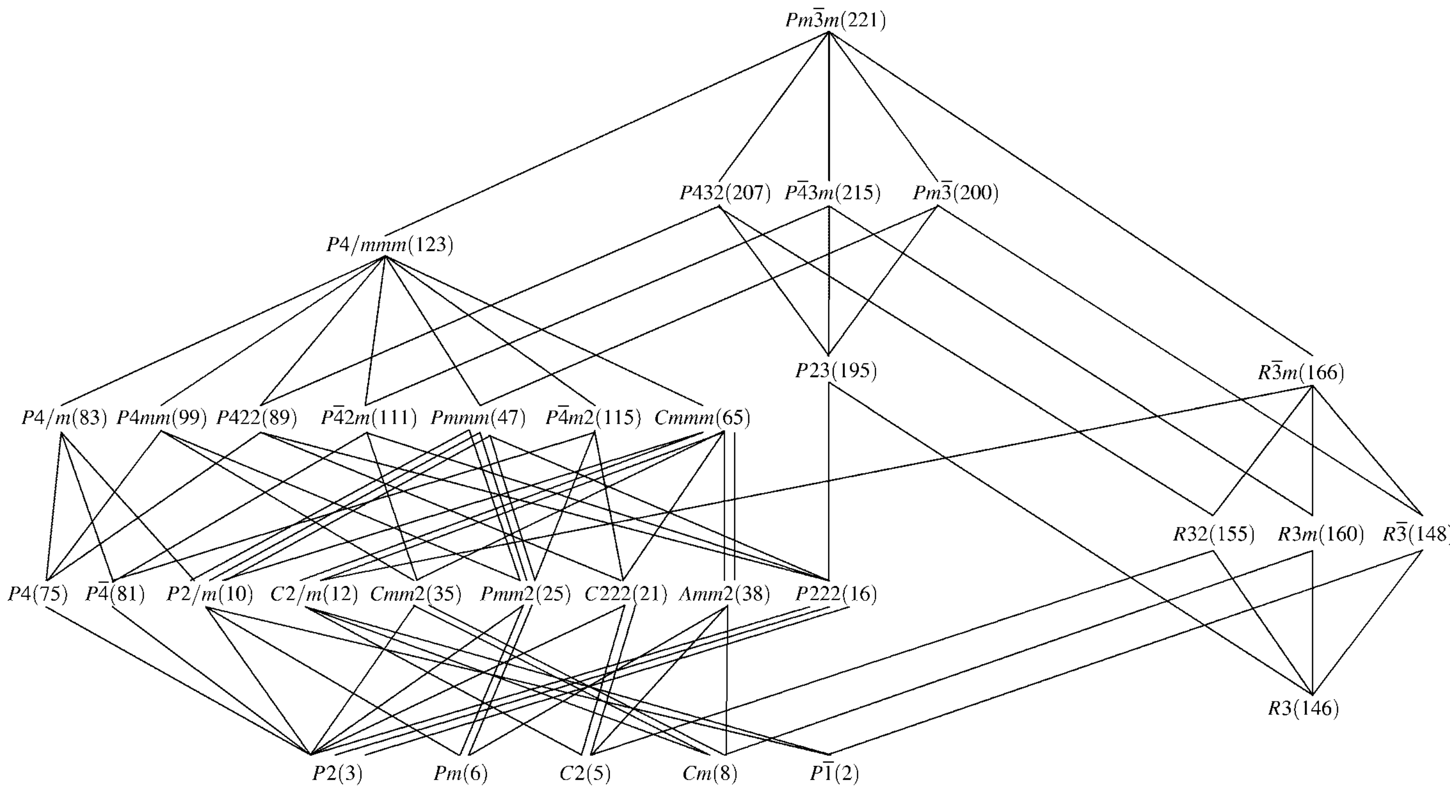

Fig. 2.4.1.1. Graph of the *translationengleiche* subgroups of the space group $Pm\bar{3}m$.

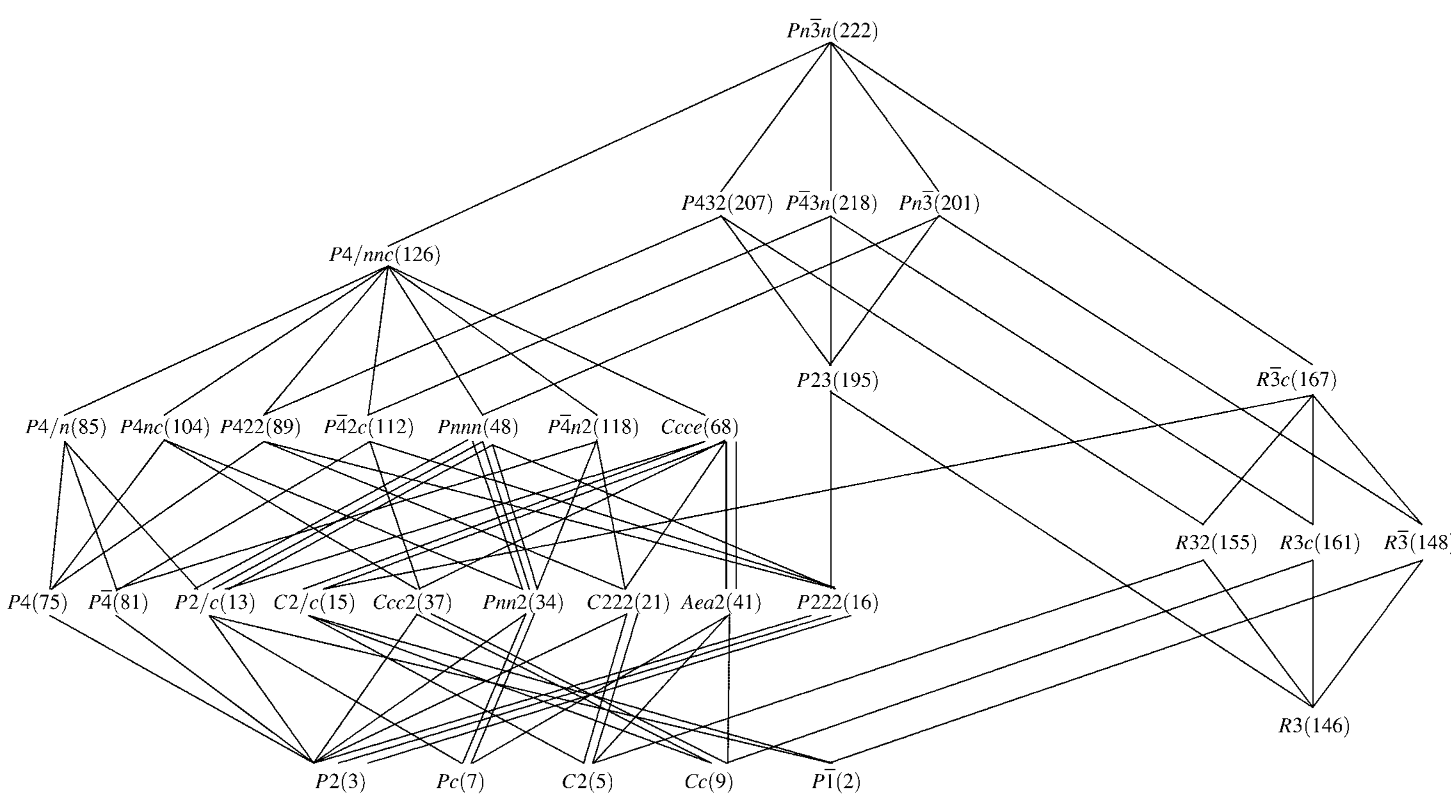

Fig. 2.4.1.2. Graph of the *translationengleiche* subgroups of the space group $Pn\bar{3}n$.

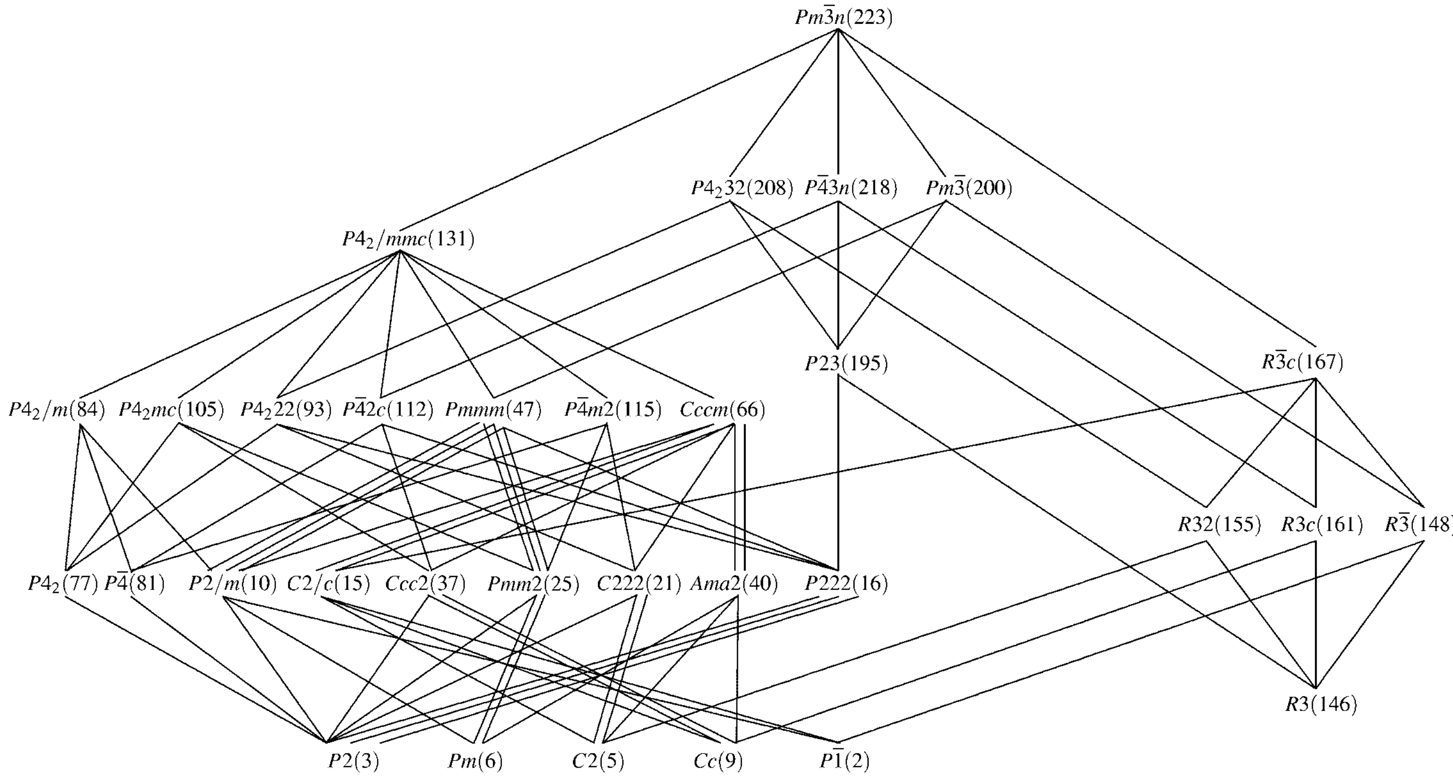

Fig. 2.4.1.3. Graph of the *translationengleiche* subgroups of the space group $Pm\bar{3}n$.

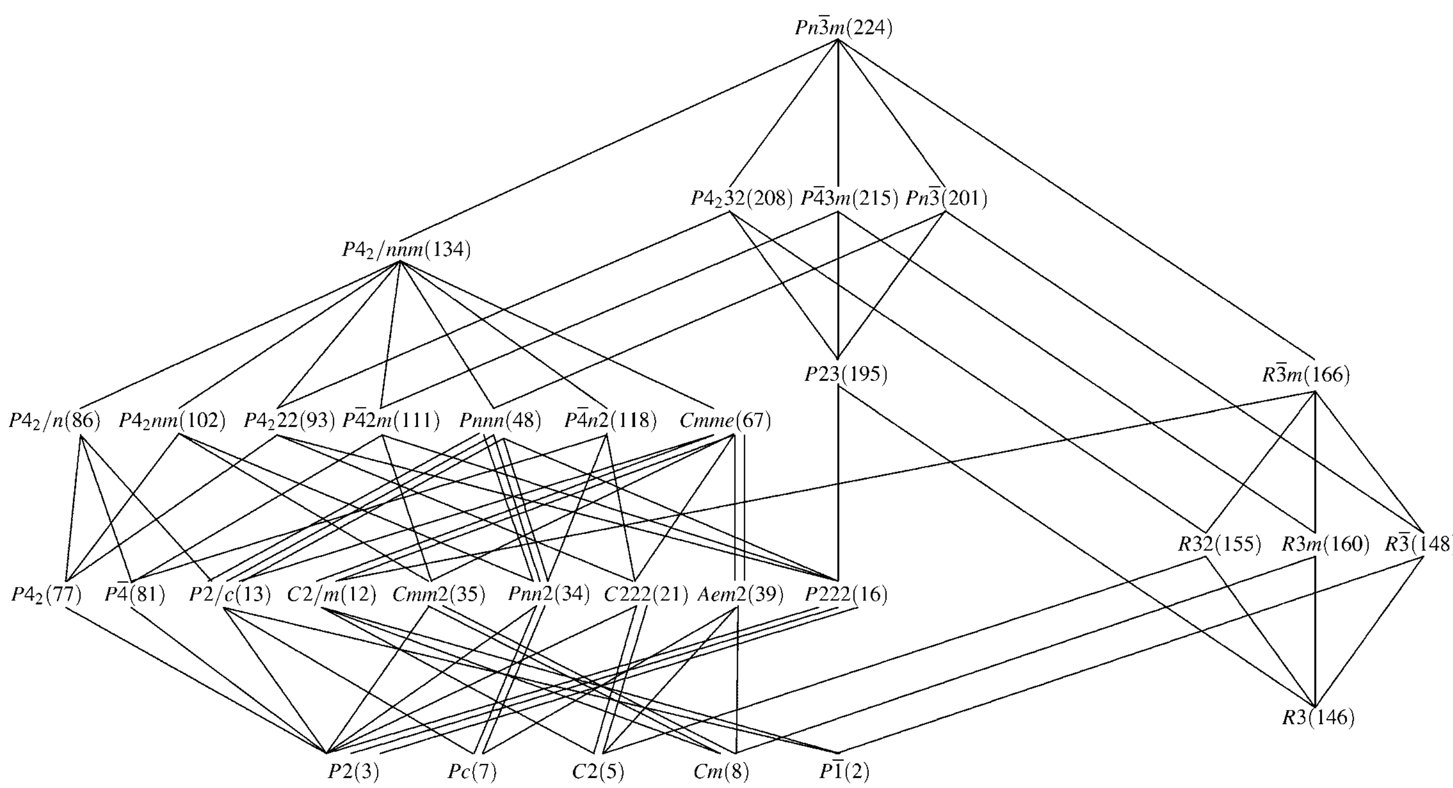

Fig. 2.4.1.4. Graph of the *translationengleiche* subgroups of the space group $Pn\bar{3}m$.

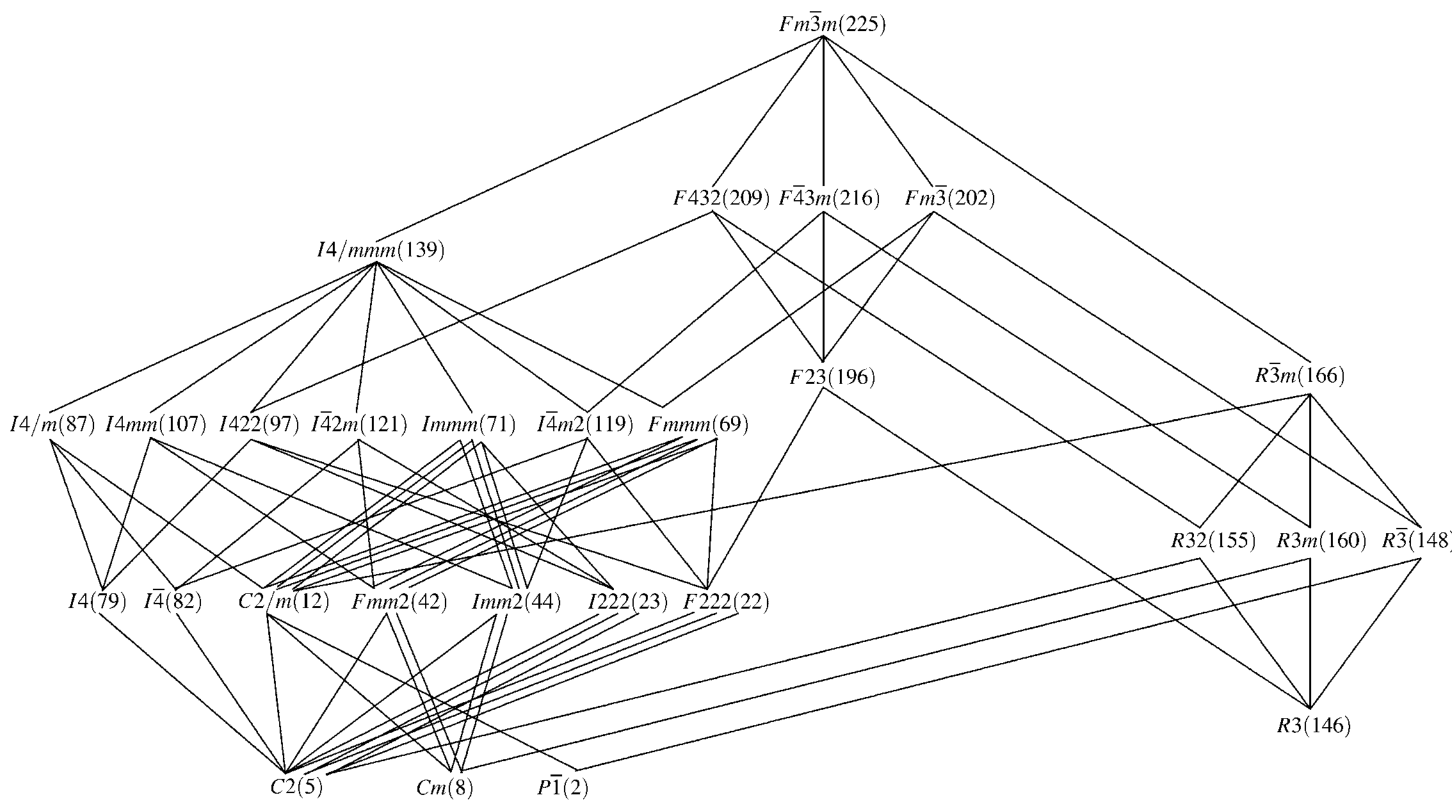

Fig. 2.4.1.5. Graph of the *translationengleiche* subgroups of the space group $Fm\bar{3}m$.

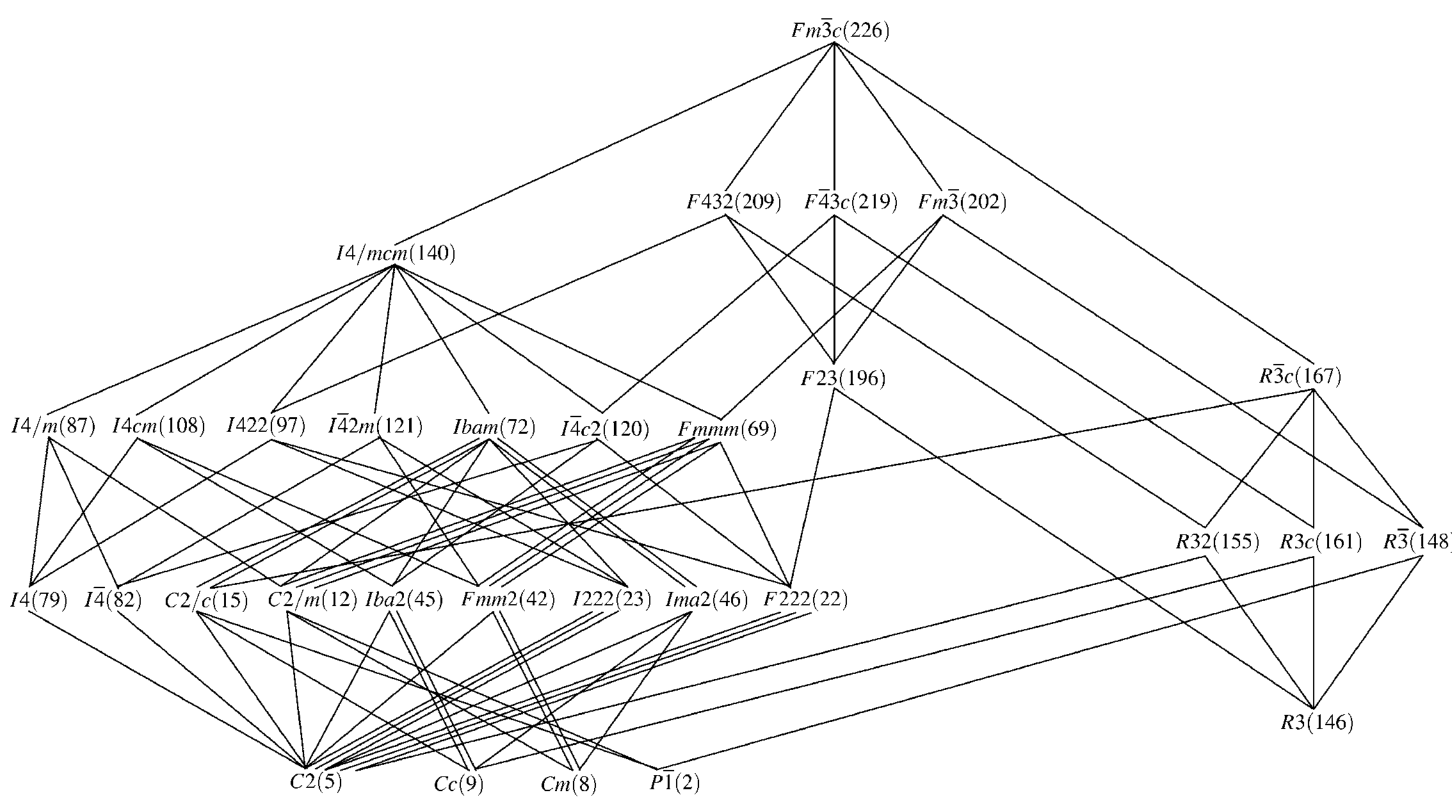

Fig. 2.4.1.6. Graph of the *translationengleiche* subgroups of the space group $Fm\bar{3}c$.

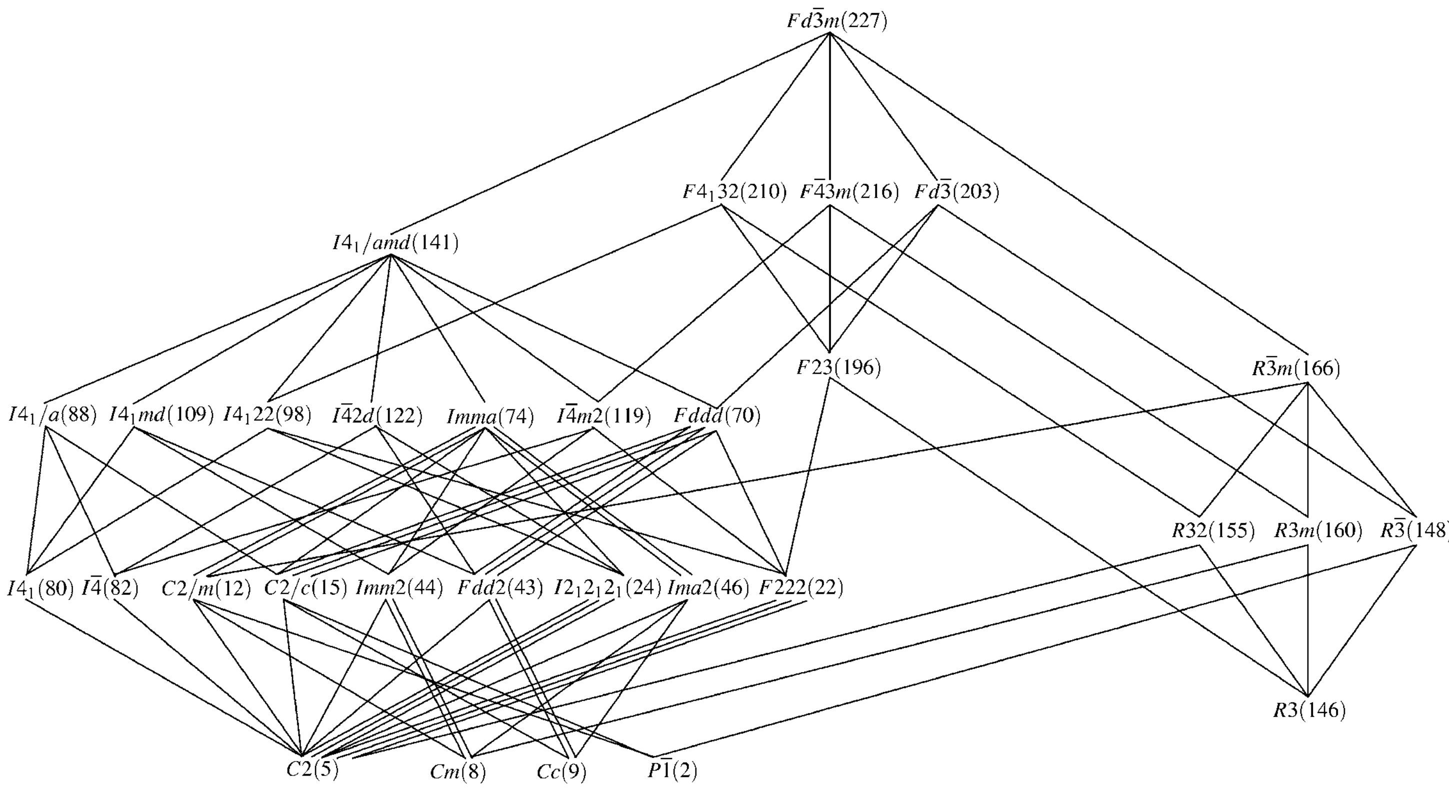

Fig. 2.4.1.7. Graph of the *translationengleiche* subgroups of the space group $Fd\bar{3}m$.

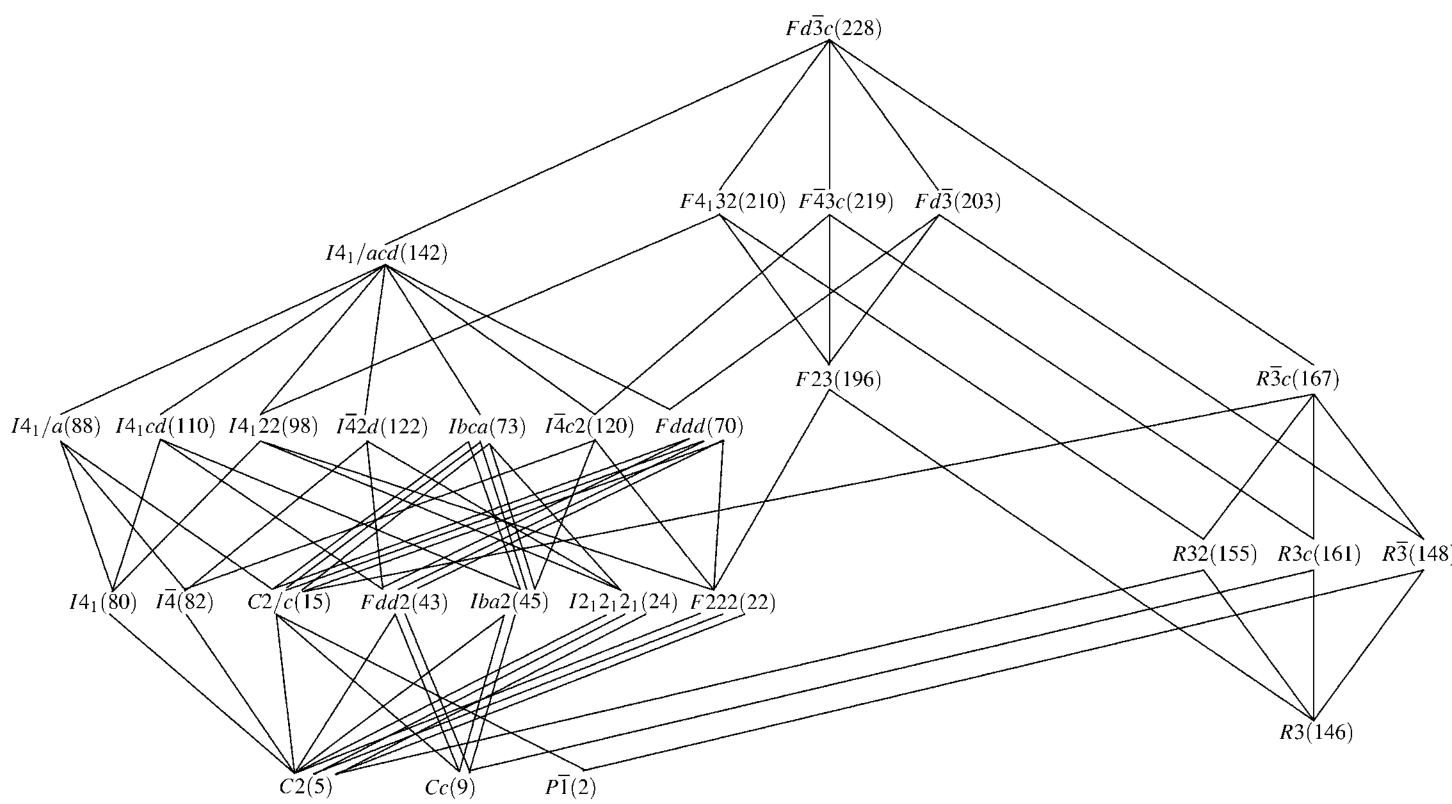

Fig. 2.4.1.8. Graph of the *translationengleiche* subgroups of the space group $Fd\bar{3}c$.

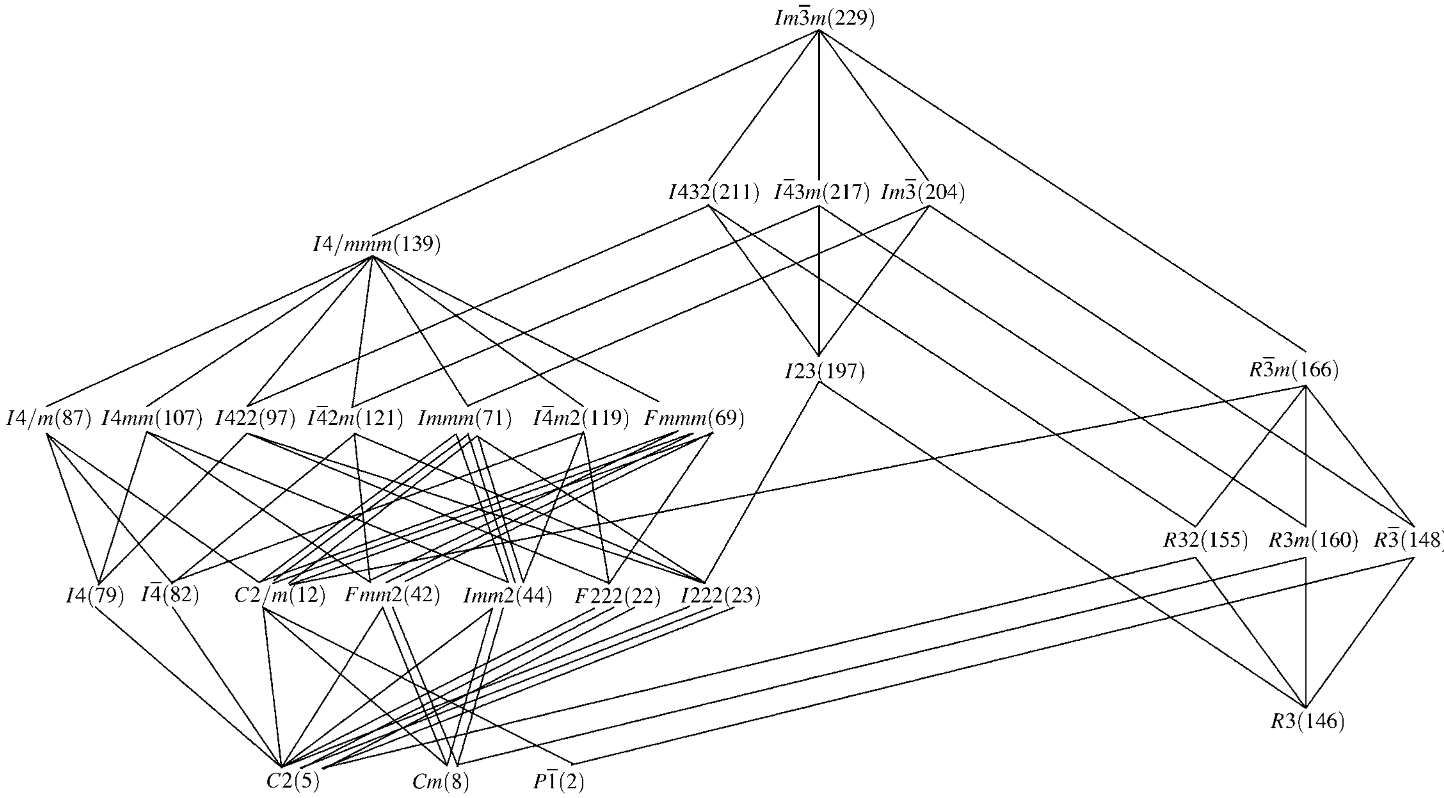

Fig. 2.4.1.9. Graph of the *translationengleiche* subgroups of the space group $Im\bar{3}m$.

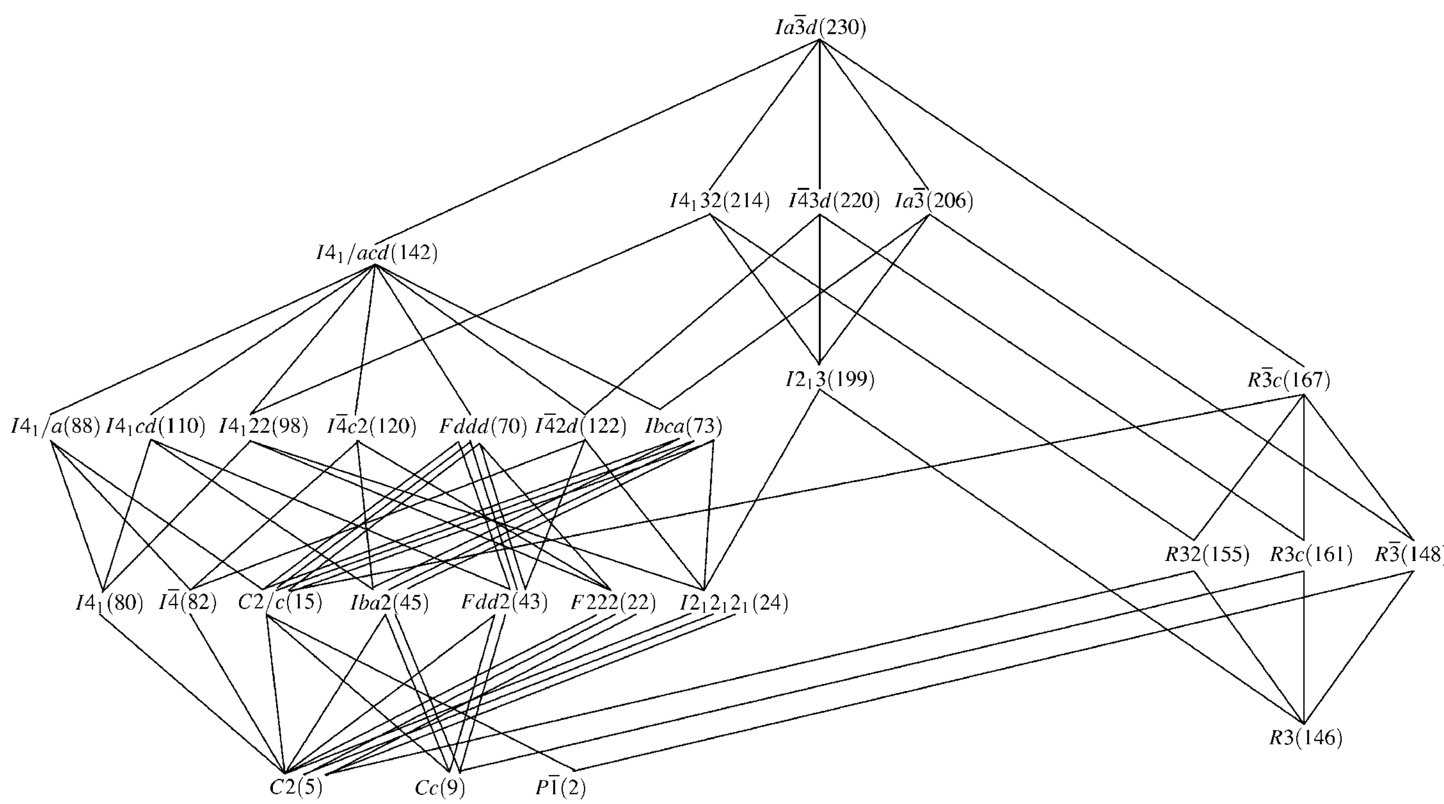

Fig. 2.4.1.10. Graph of the *translationengleiche* subgroups of the space group $Ia\bar{3}d$.

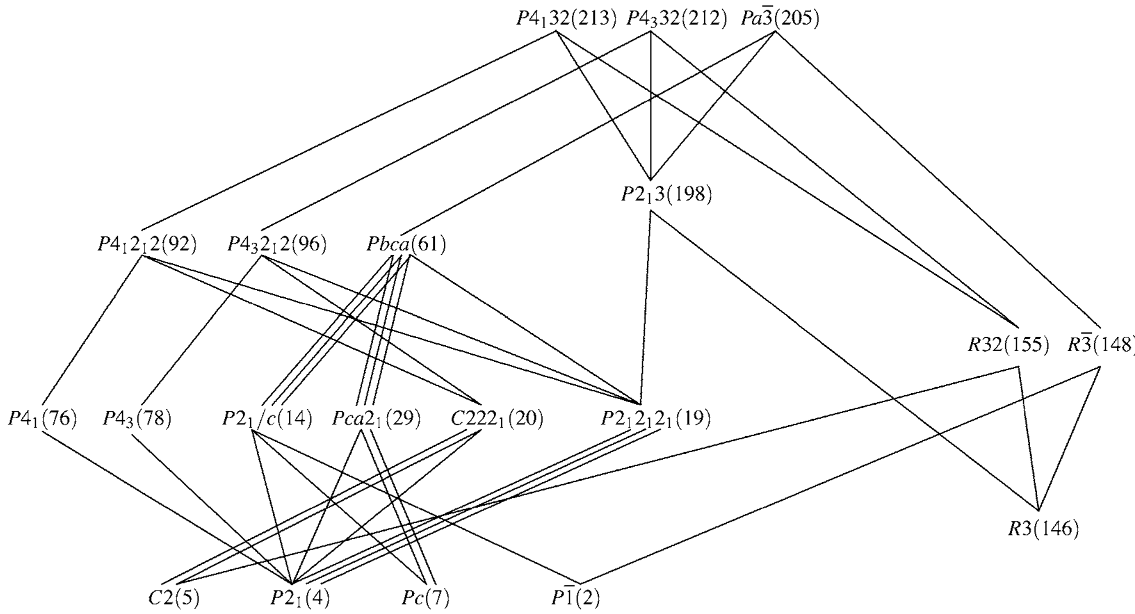

Fig. 2.4.1.11. Graph of the *translationengleiche* subgroups of the space groups $P4_132$, $P4_332$ and $Pa\bar{3}$.

2.4.2. Graphs of the *translationengleiche* subgroups with a tetragonal summit

For an explanation of these graphs, see Section 2.1.7.2 (p. 54).

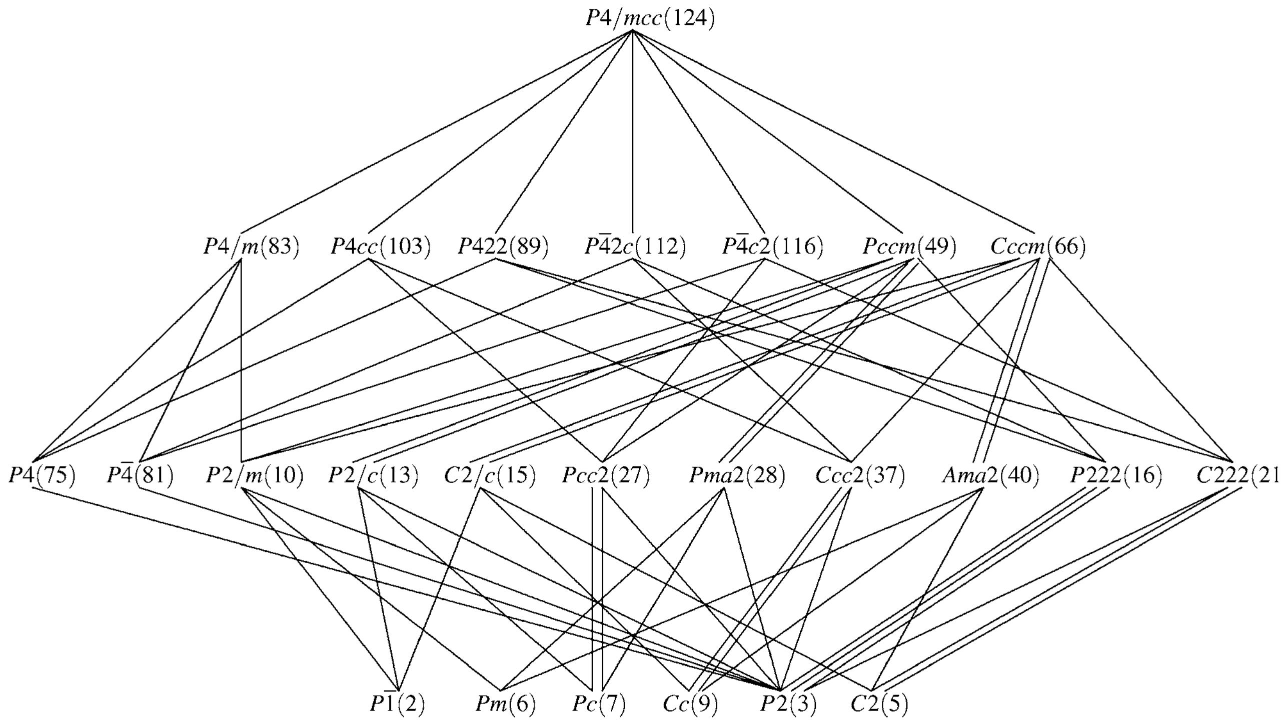

Fig. 2.4.2.1. Graph of the *translationengleiche* subgroups of the space group $P4/mcc$.

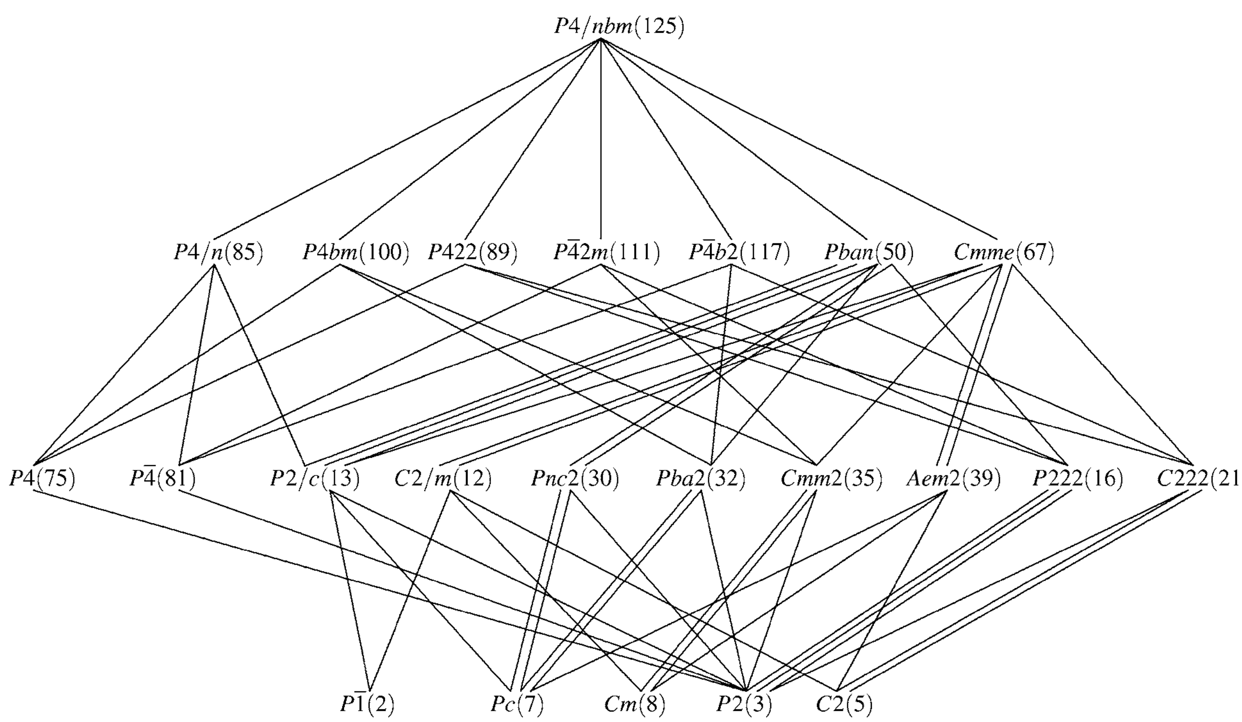

Fig. 2.4.2.2. Graph of the *translationengleiche* subgroups of the space group $P4/nbm$.

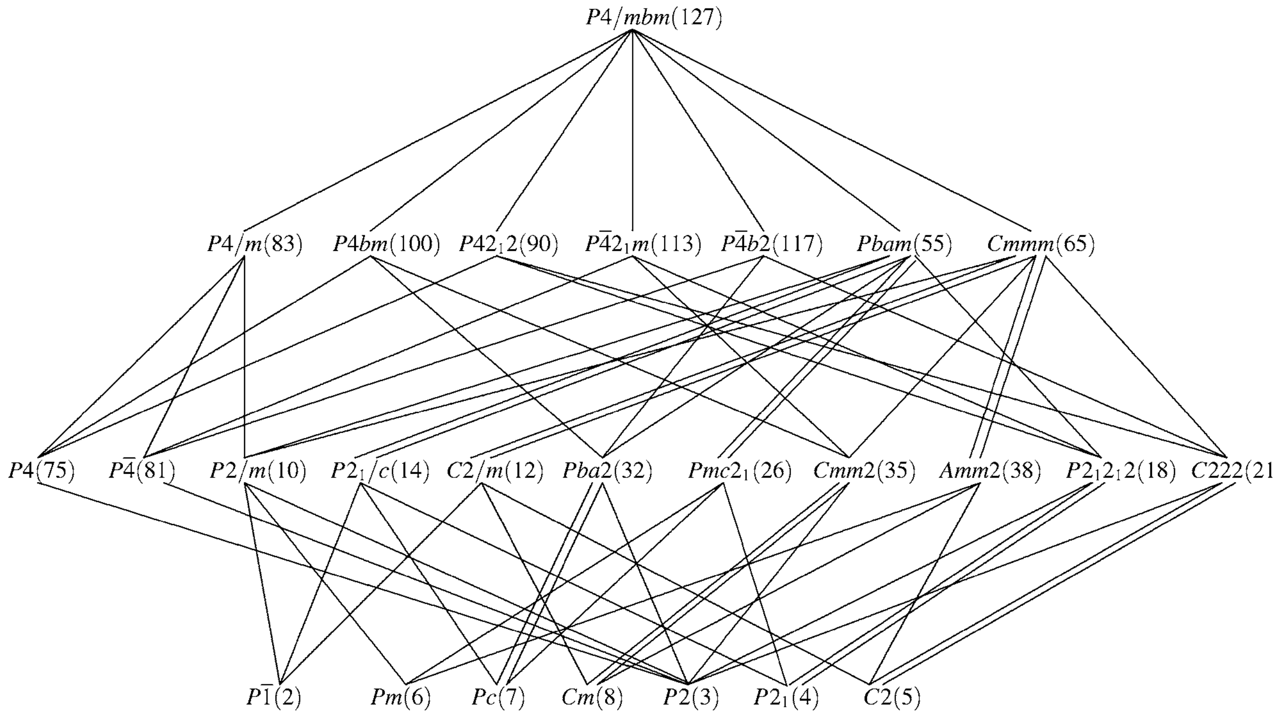

Fig. 2.4.2.3. Graph of the *translationengleiche* subgroups of the space group $P4/mbm$.

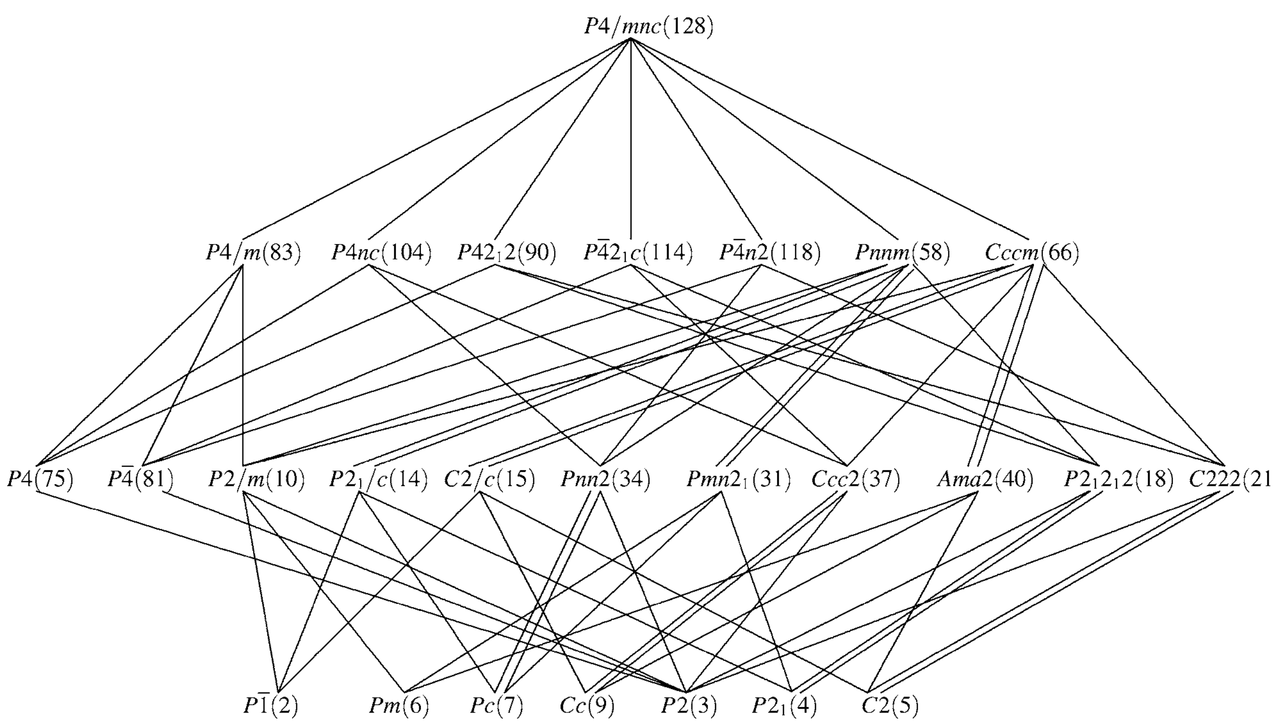

Fig. 2.4.2.4. Graph of the *translationengleiche* subgroups of the space group $P4/mnc$.

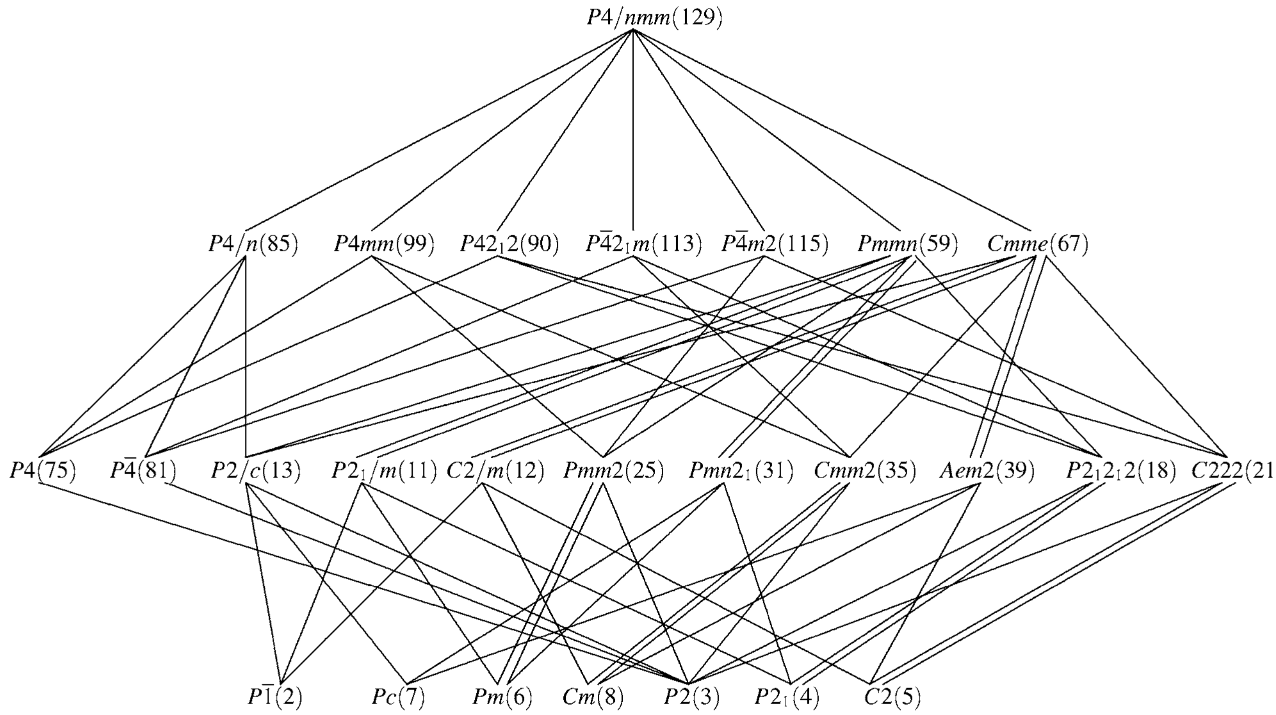

Fig. 2.4.2.5. Graph of the *translationengleiche* subgroups of the space group $P4/nmm$.

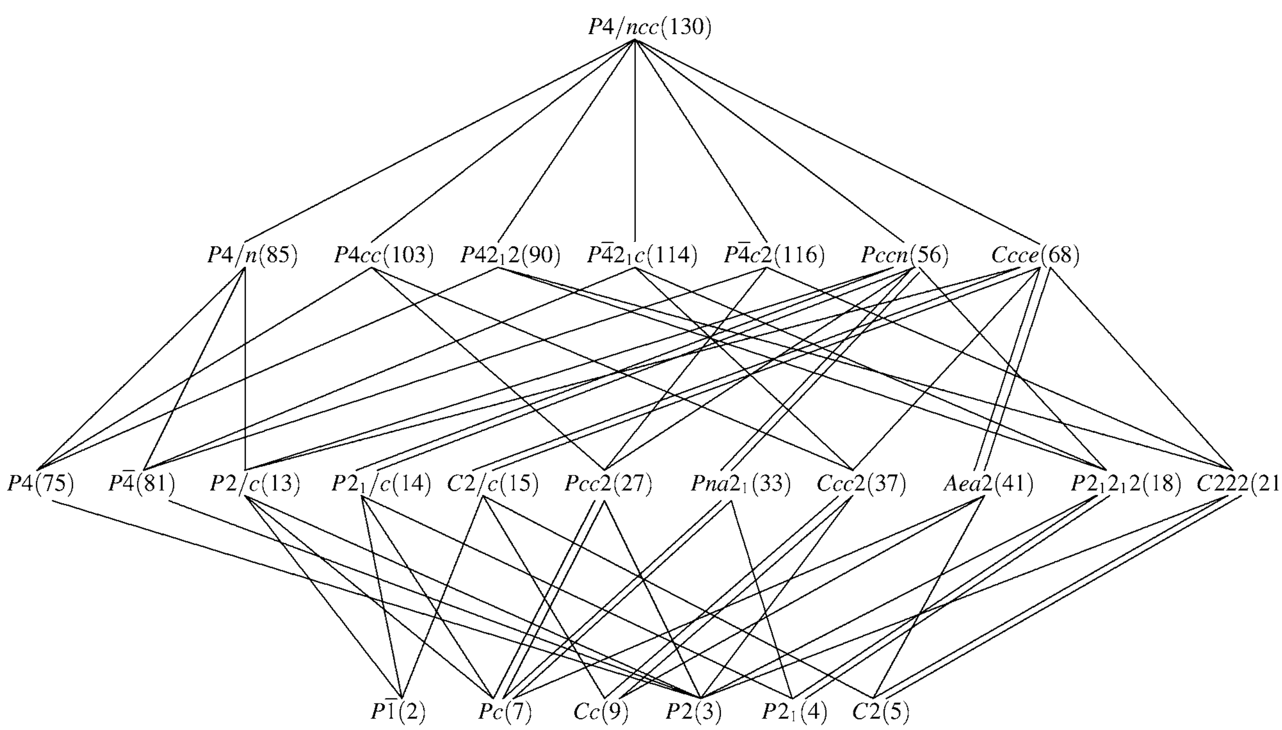

Fig. 2.4.2.6. Graph of the *translationengleiche* subgroups of the space group $P4/ncc$.

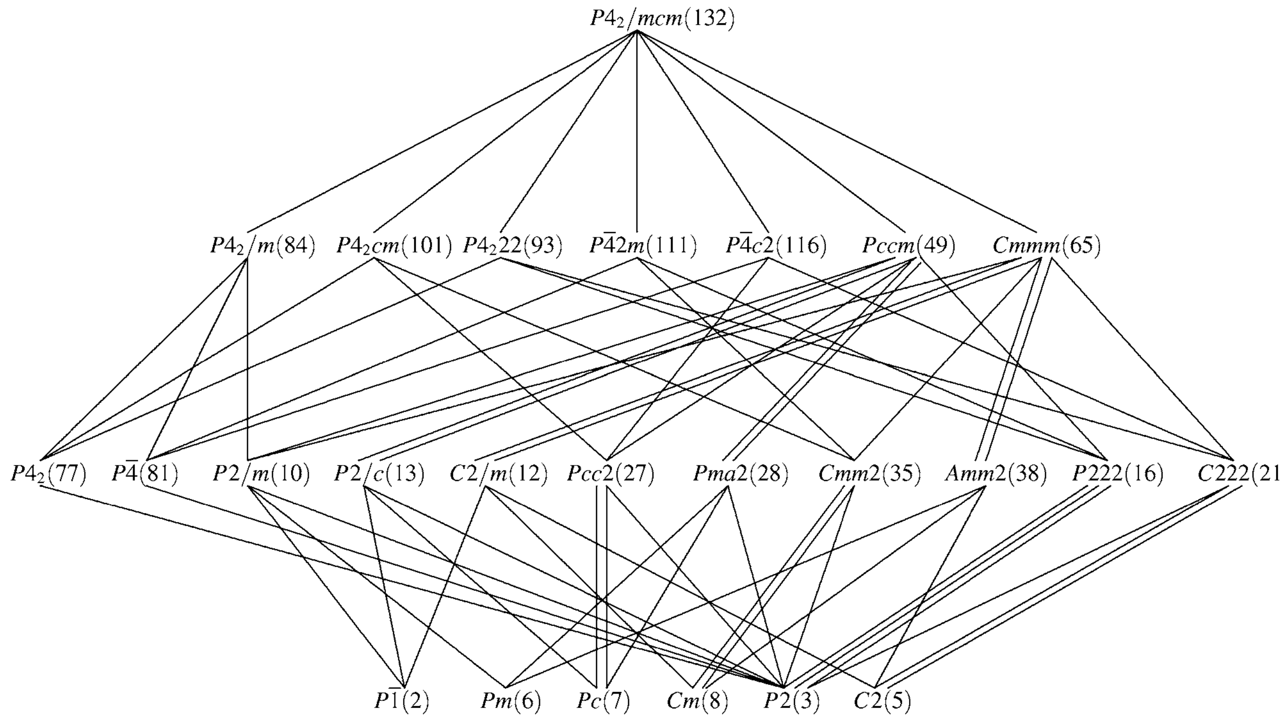

Fig. 2.4.2.7. Graph of the *translationengleiche* subgroups of the space group $P4_2/mcm$.

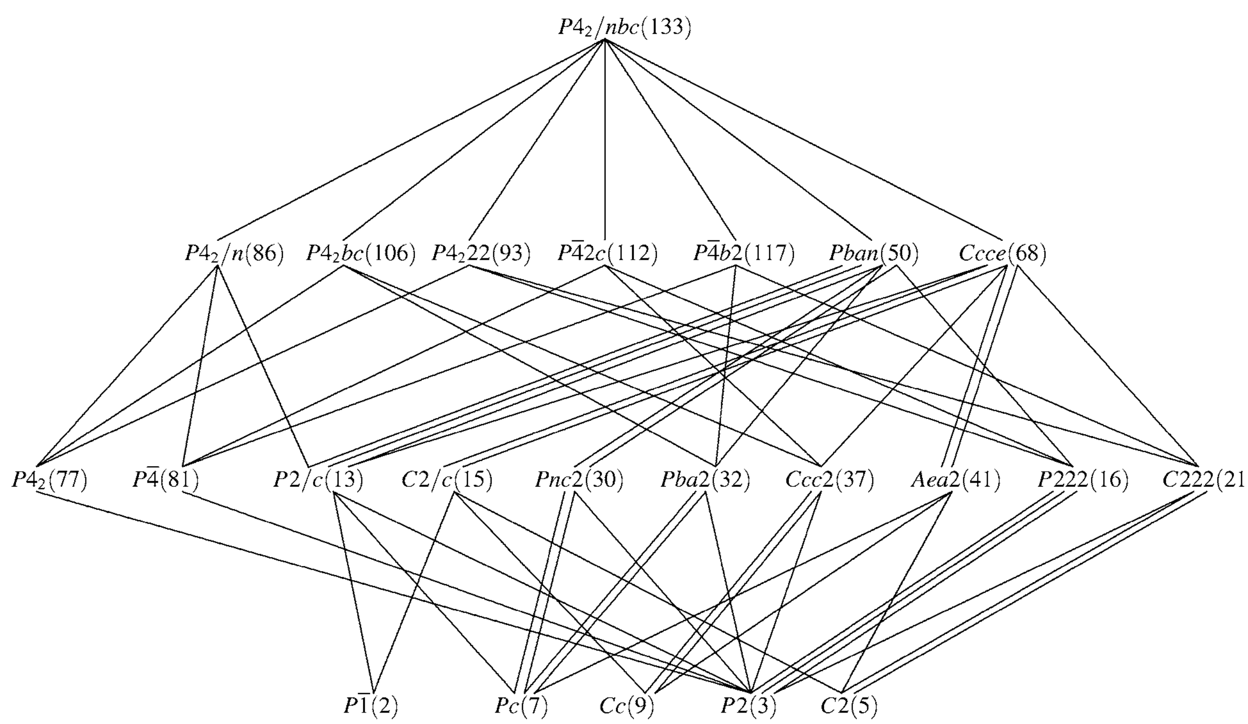

Fig. 2.4.2.8. Graph of the *translationengleiche* subgroups of the space group $P4_2/nbc$.

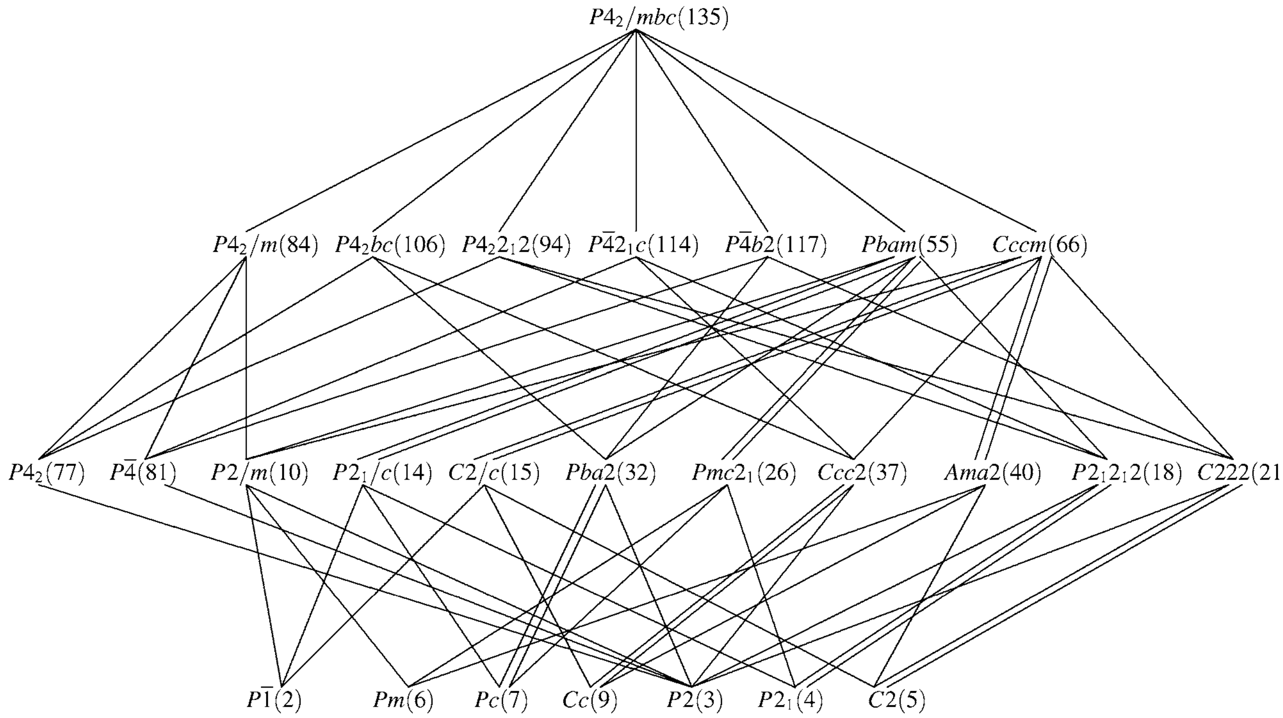

Fig. 2.4.2.9. Graph of the *translationengleiche* subgroups of the space group $P4_2/mbc$.

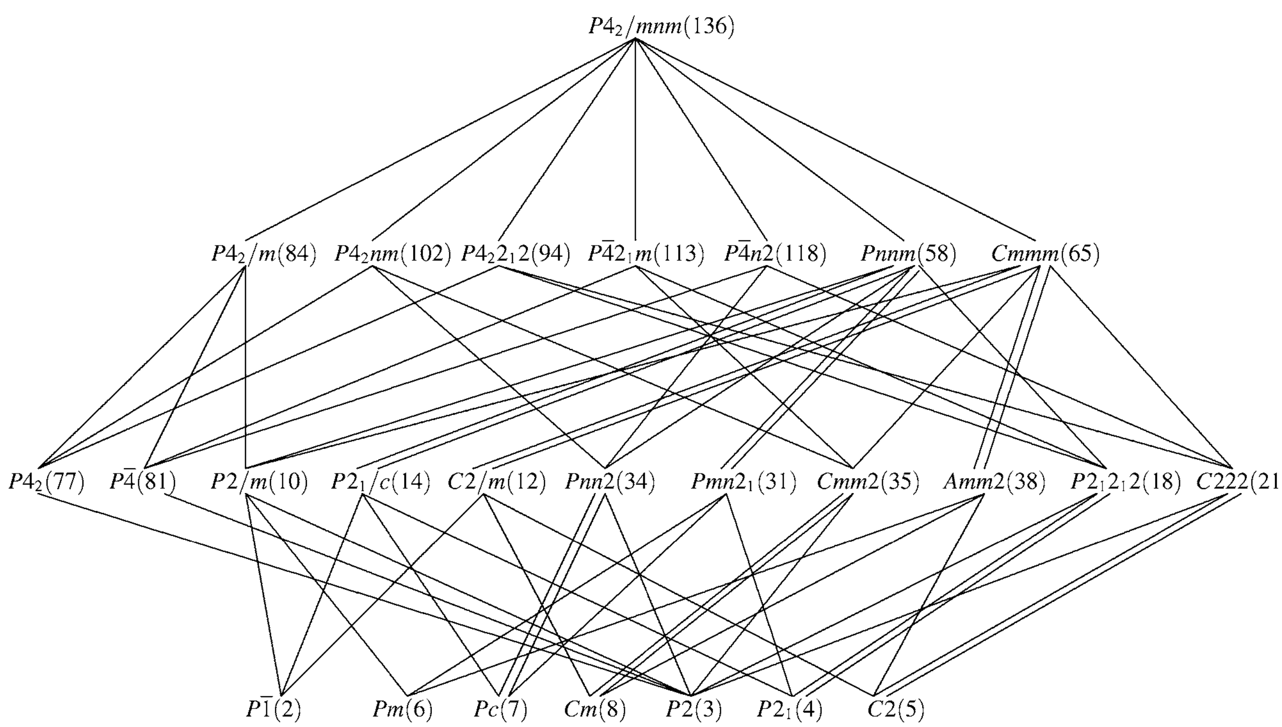

Fig. 2.4.2.10. Graph of the *translationengleiche* subgroups of the space group $P4_2/mnm$.

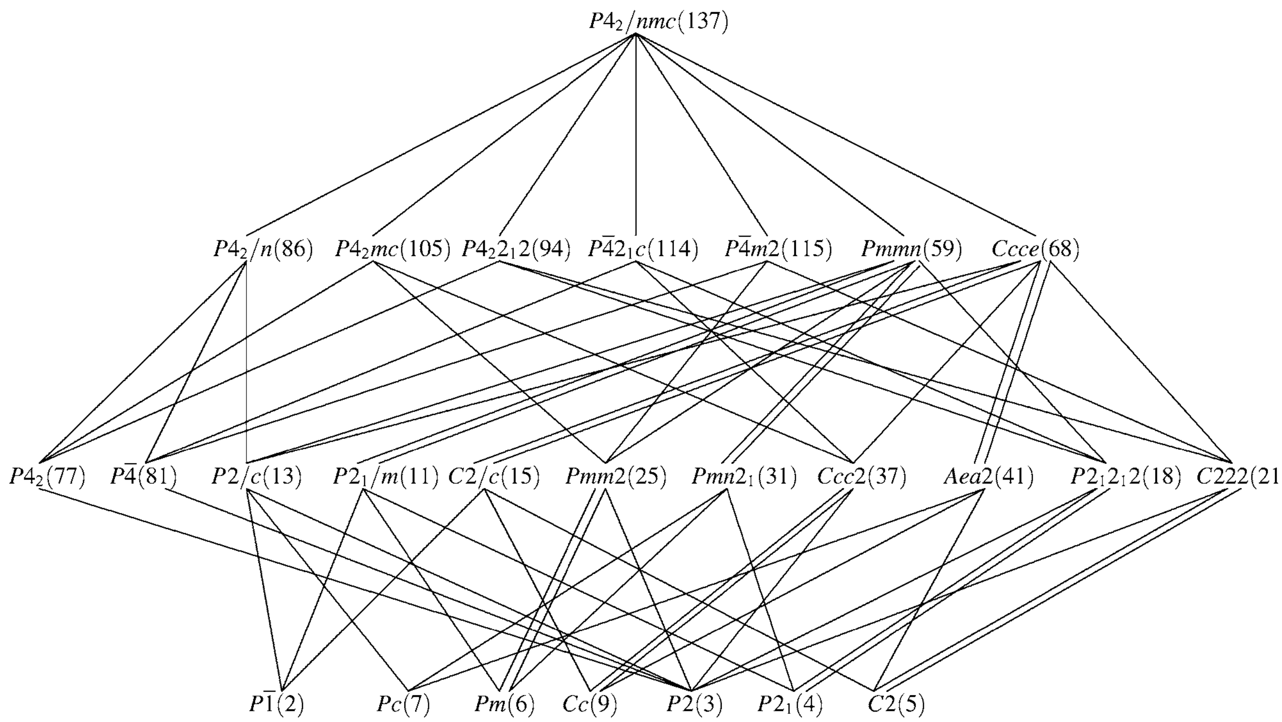

Fig. 2.4.2.11. Graph of the *translationengleiche* subgroups of the space group $P4_2/nmc$.

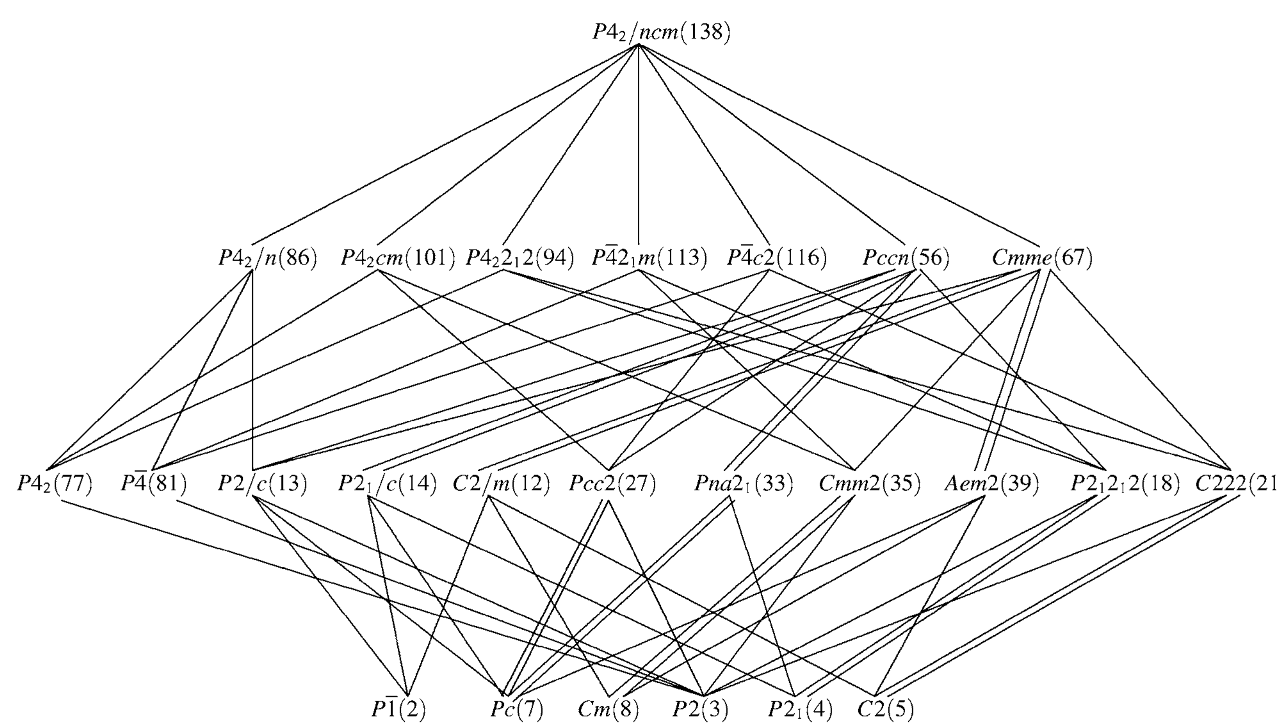

Fig. 2.4.2.12. Graph of the *translationengleiche* subgroups of the space group $P4_2/ncm$.

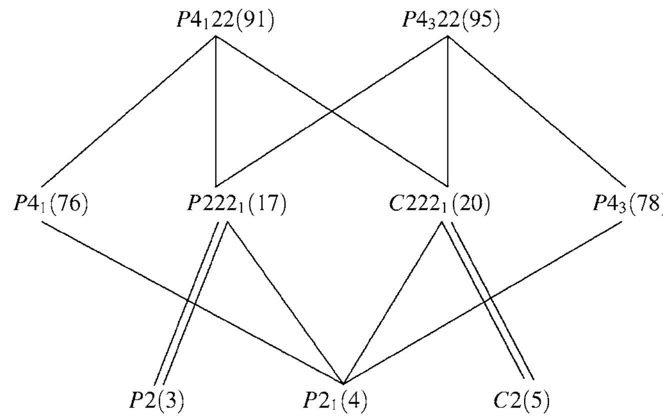

Fig. 2.4.2.13. Graph of the *translationengleiche* subgroups of the space groups $P4_122$ and $P4_322$.

2.4.3. Graphs of the *translationengleiche* subgroups with a hexagonal summit

For an explanation of these graphs, see Section 2.1.7.2 (p. 54).

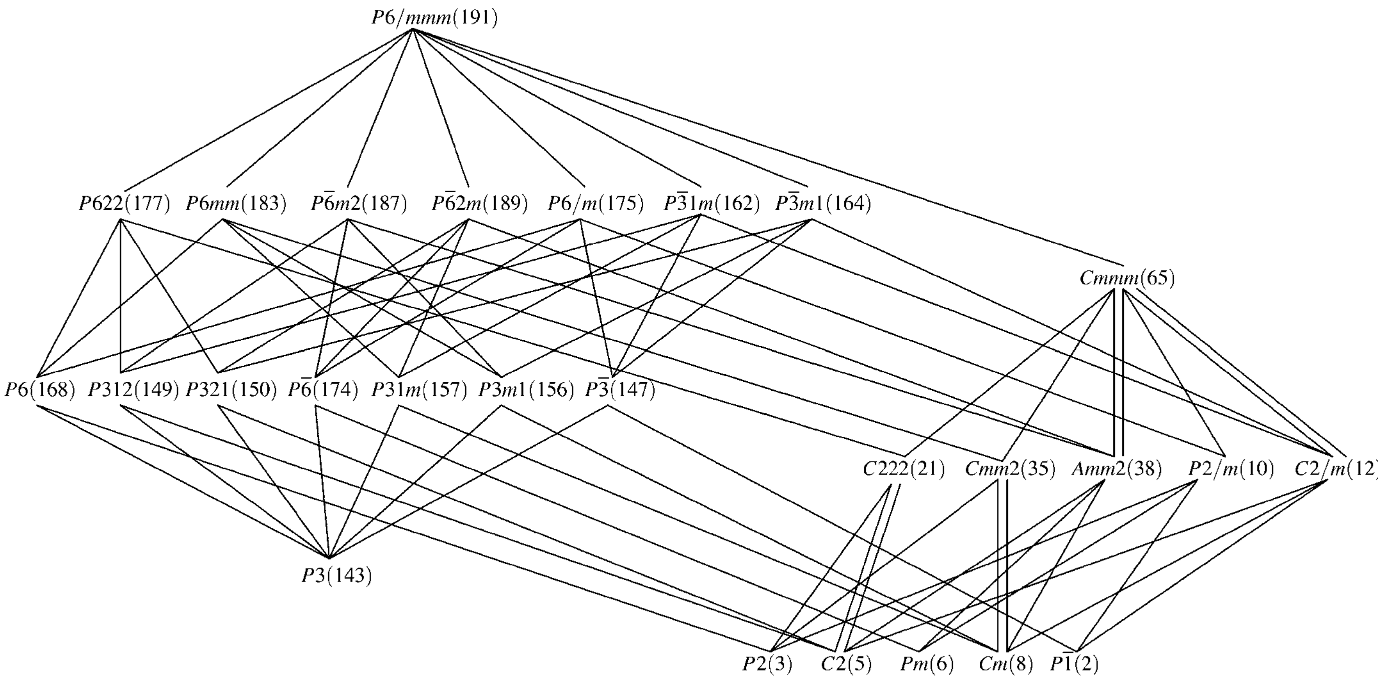

Fig. 2.4.3.1. Graph of the *translationengleiche* subgroups of the space group $P6/mmm$.

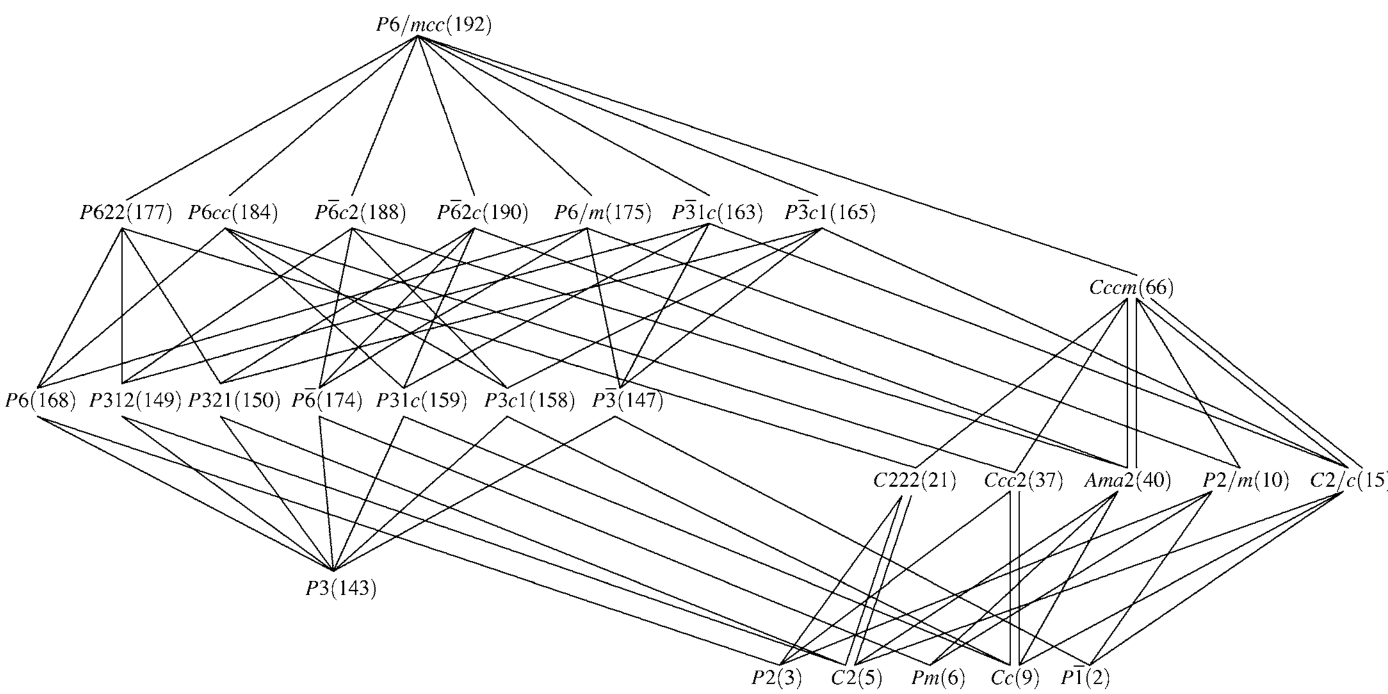

Fig. 2.4.3.2. Graph of the *translationengleiche* subgroups of the space group $P6/mcc$.

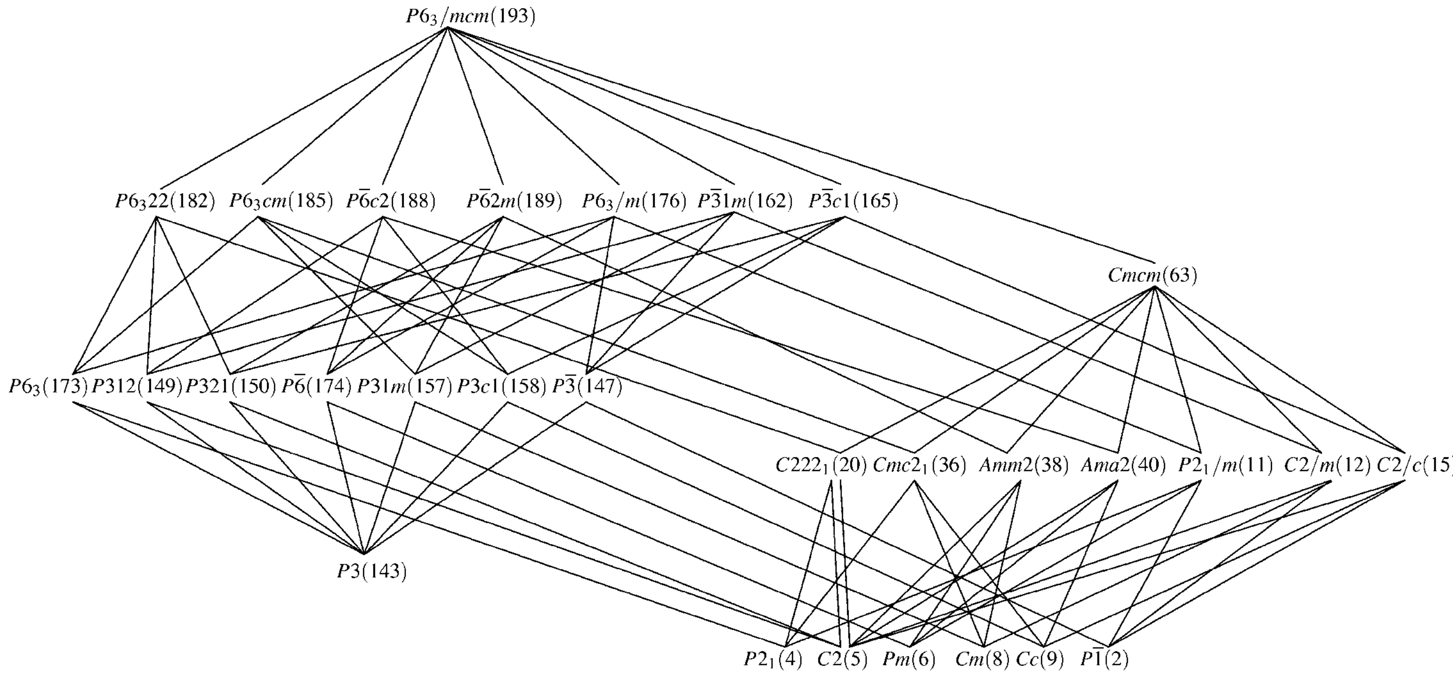

Fig. 2.4.3.3. Graph of the *translationengleiche* subgroups of the space group $P6_3/mcm$.

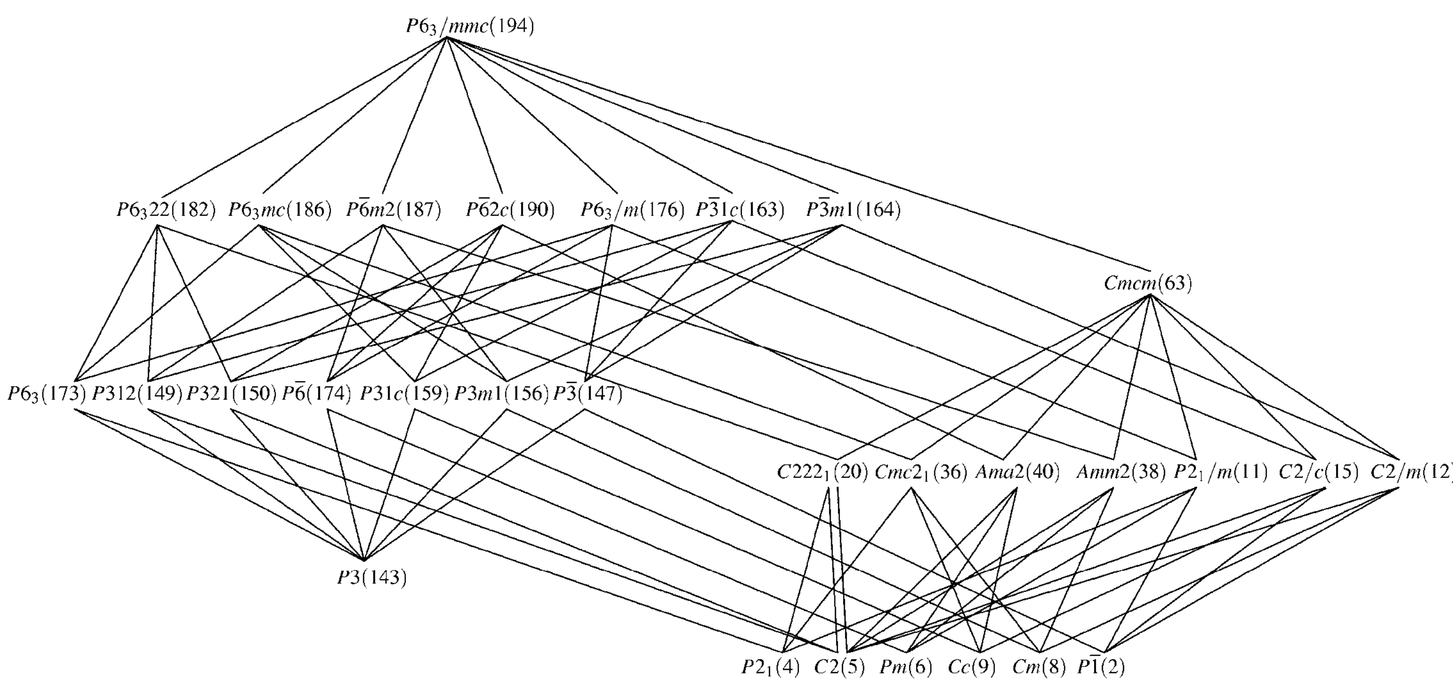

Fig. 2.4.3.4. Graph of the *translationengleiche* subgroups of the space group $P6_3/mmc$.

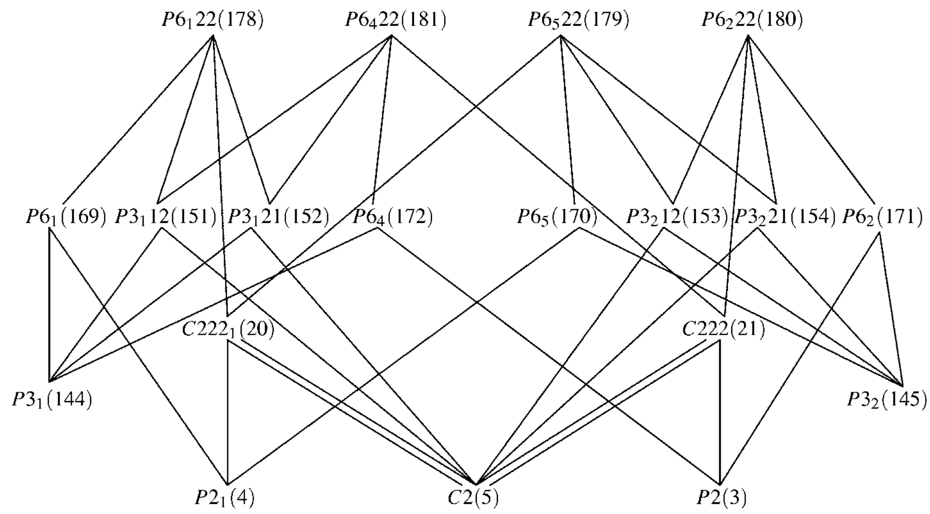

Fig. 2.4.3.5. Graph of the *translationengleiche* subgroups of the space groups $P6_122$, $P6_522$, $P6_222$ and $P6_422$.

2.4.4. Graphs of the *translationengleiche* subgroups with an orthorhombic summit

For an explanation of these graphs, see Section 2.1.7.2 (p. 54).

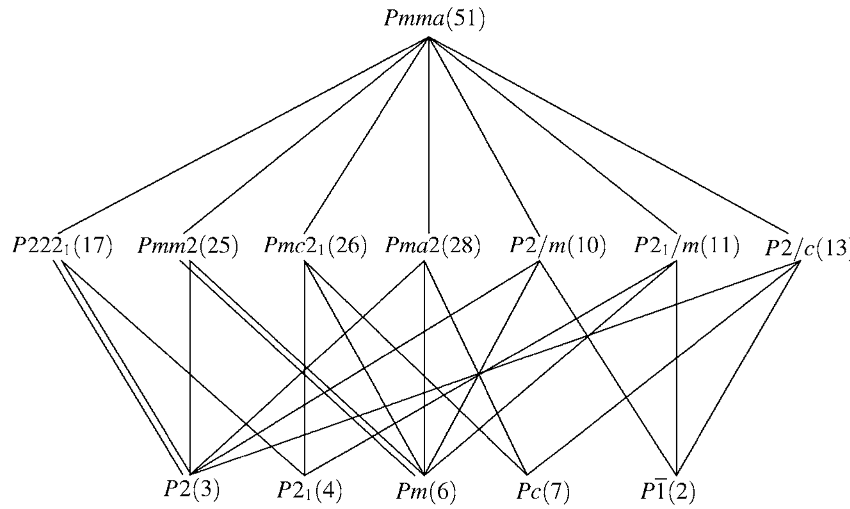

Fig. 2.4.4.1. Graph of the *translationengleiche* subgroups of the space group *Pmma*.

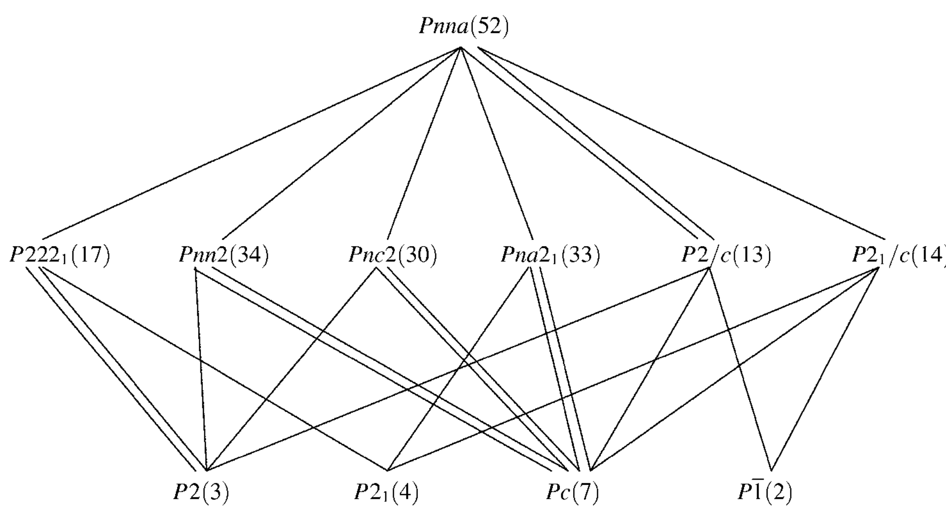

Fig. 2.4.4.2. Graph of the *translationengleiche* subgroups of the space group *Pnna*.

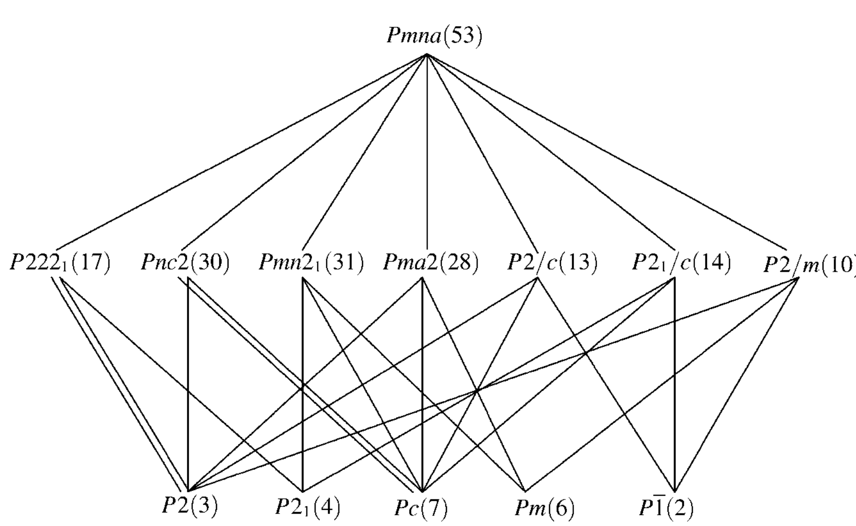

Fig. 2.4.4.3. Graph of the *translationengleiche* subgroups of the space group *Pmna*.

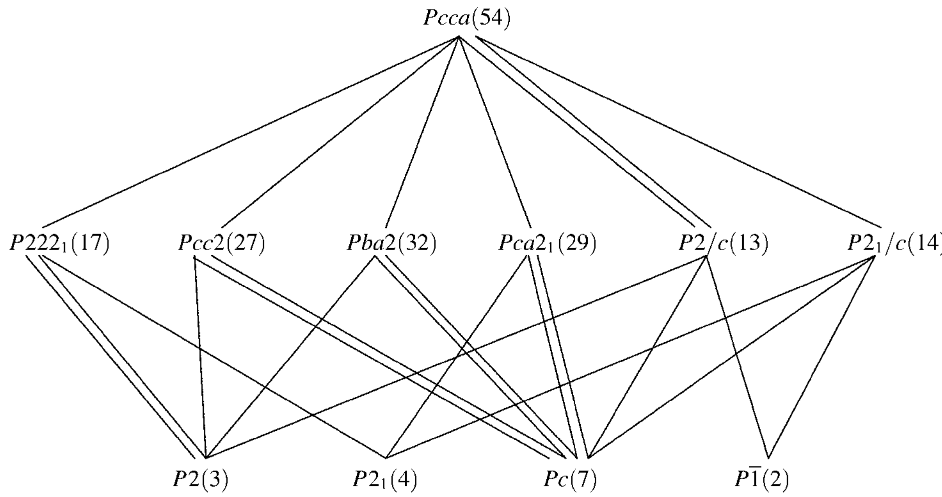

Fig. 2.4.4.4. Graph of the *translationengleiche* subgroups of the space group *Pcca*.

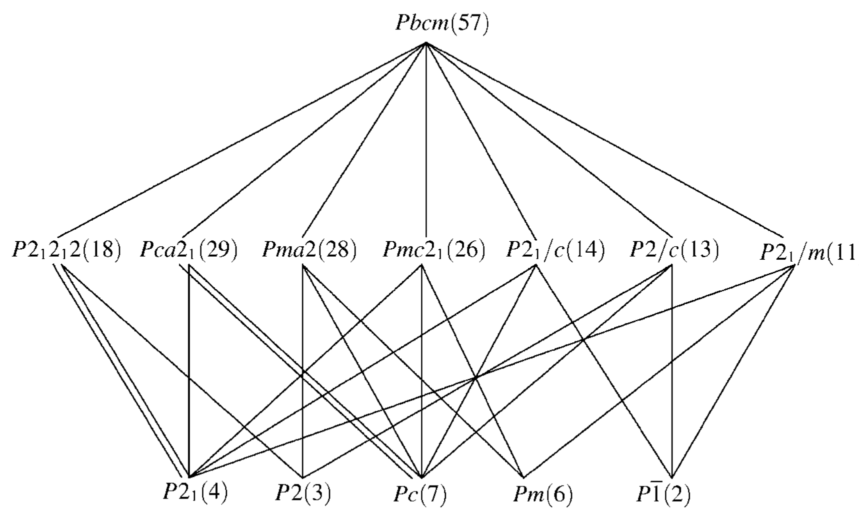

Fig. 2.4.4.5. Graph of the *translationengleiche* subgroups of the space group *Pbcm*.

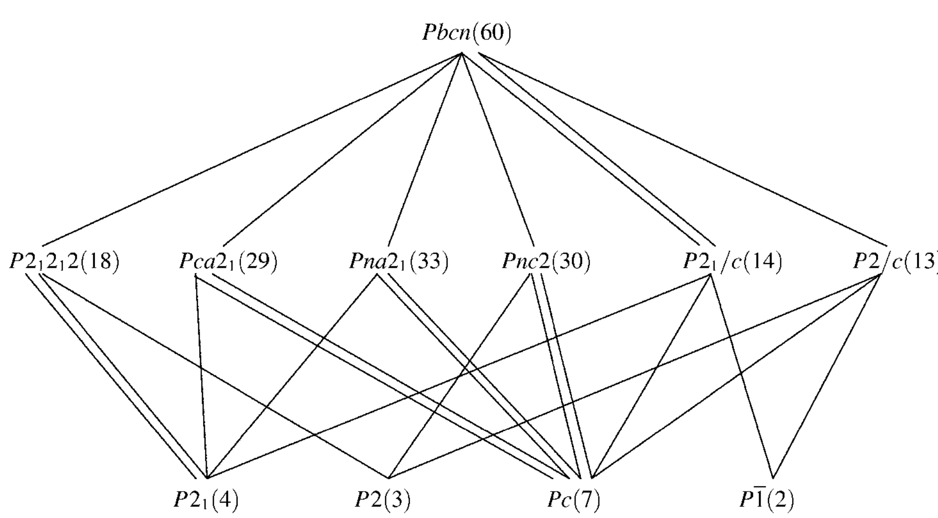

Fig. 2.4.4.6. Graph of the *translationengleiche* subgroups of the space group *Pbcn*.

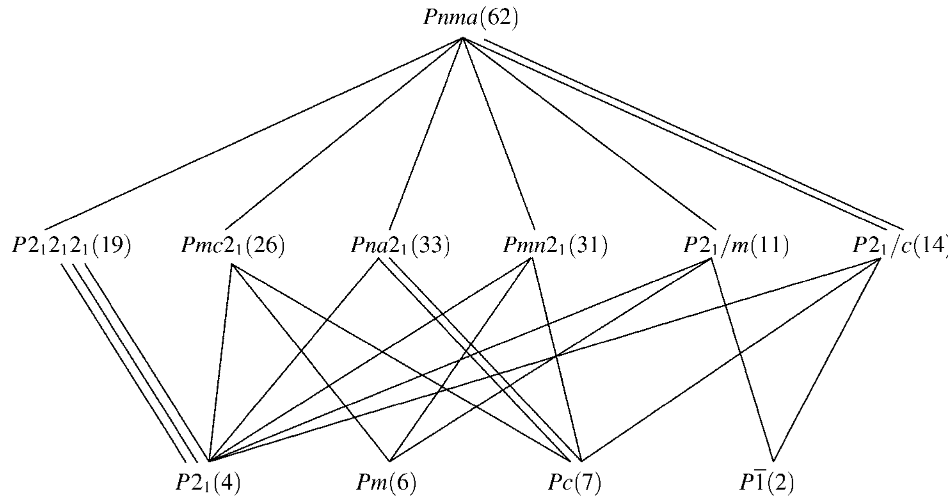

Fig. 2.4.4.7. Graph of the *translationengleiche* subgroups of the space group *Pnma*.

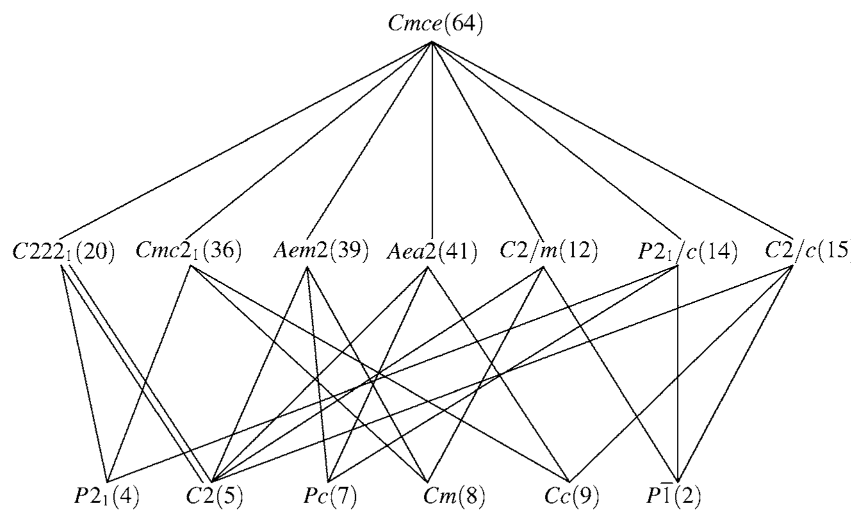

Fig. 2.4.4.8. Graph of the *translationengleiche* subgroups of the space group *Cmce*.

references

International Tables for Crystallography (2006). Vol. A1, Chapter 2.5, pp. 415–425.

2.5. Graphs for *klassengleiche* subgroups

BY VOLKER GRAMLICH AND HANS WONDRATSCHEK

2.5.1. Graphs of the *klassengleiche* subgroups of monoclinic and orthorhombic space groups

For an explanation of these graphs, see Section 2.1.7.3 (p. 55).

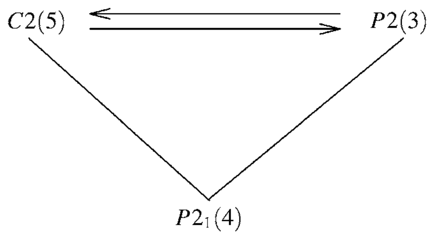

Fig. 2.5.1.1. Graph of the *klassengleiche* subgroups of the space groups of crystal class 2.

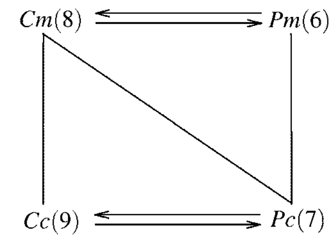

Fig. 2.5.1.2. Graph of the *klassengleiche* subgroups of the space groups of crystal class *m*.

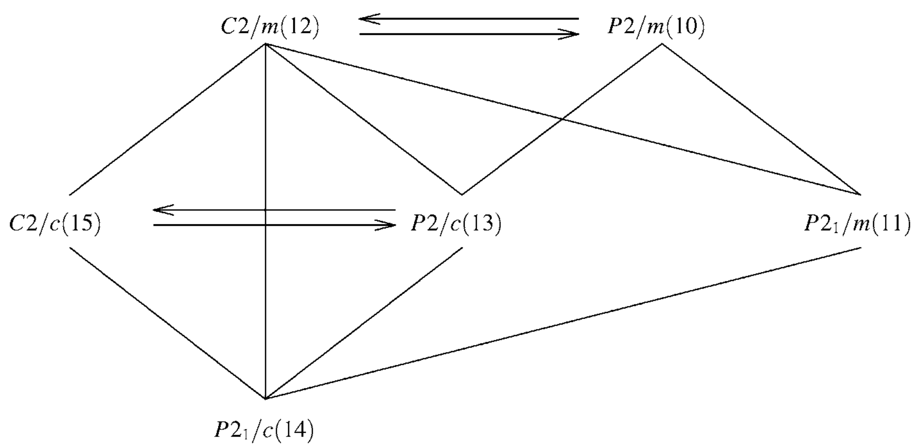

Fig. 2.5.1.3. Graph of the *klassengleiche* subgroups of the space groups of crystal class $2/m$.

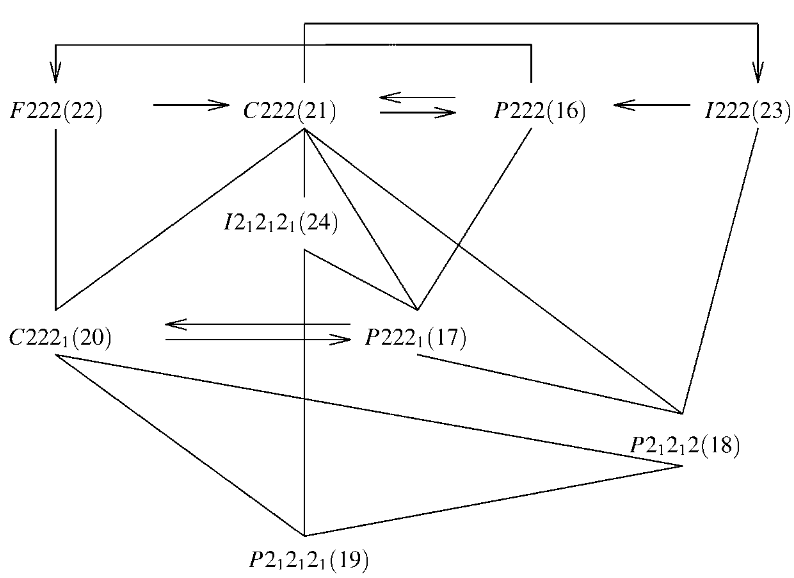

Fig. 2.5.1.4. Graph of the *klassengleiche* subgroups of the space groups of crystal class 222.

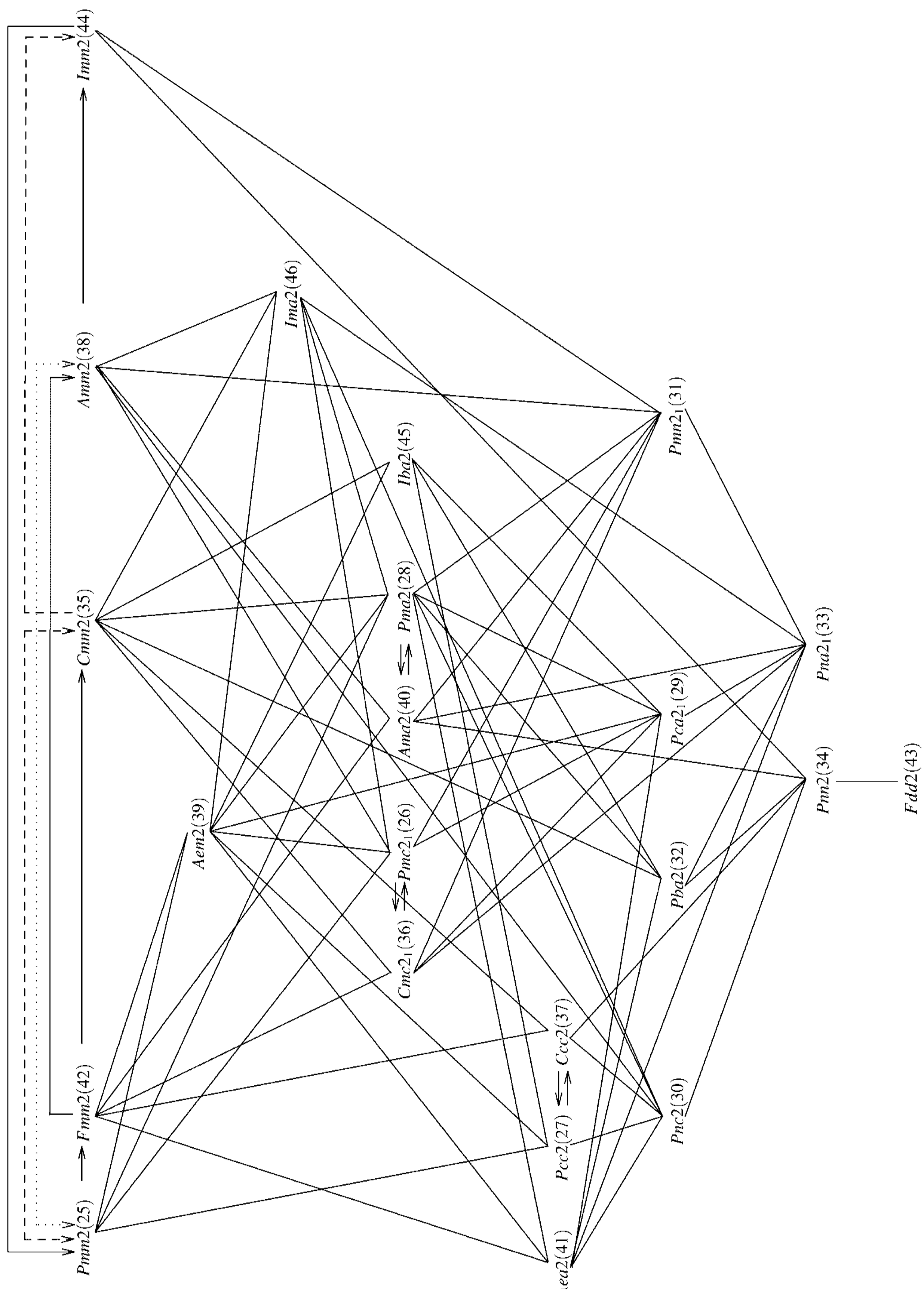

Fig. 2.5.1.5. Graph of the *klassengleiche* subgroups of the space groups of crystal class *mm*2.

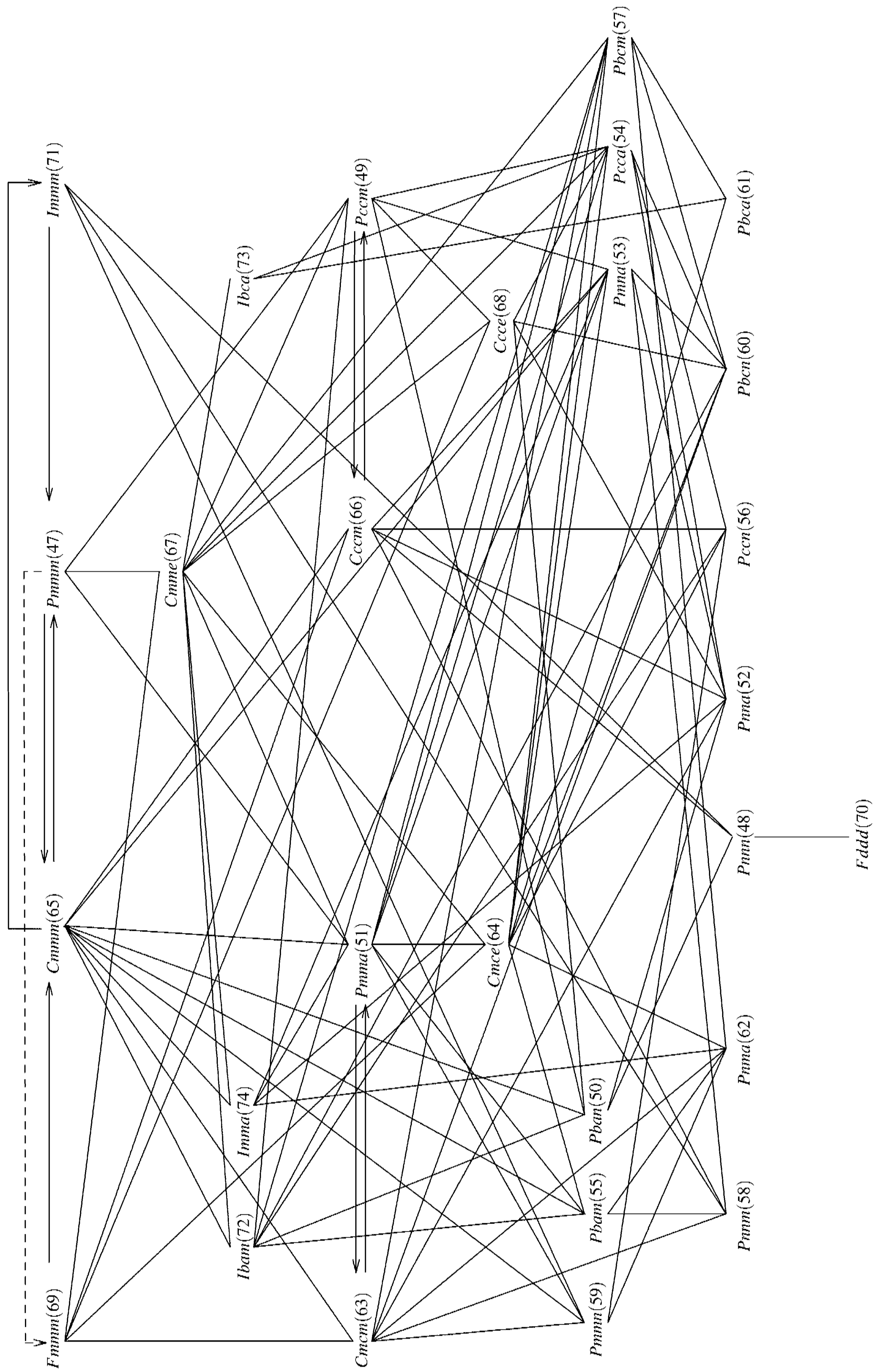

Fig. 2.5.1.6. Graph of the *klassengleiche* subgroups of the space groups of crystal class *mmm*.

2.5.2. Graphs of the *klassengleiche* subgroups of tetragonal space groups

For an explanation of these graphs, see Section 2.1.7.3 (p. 55).

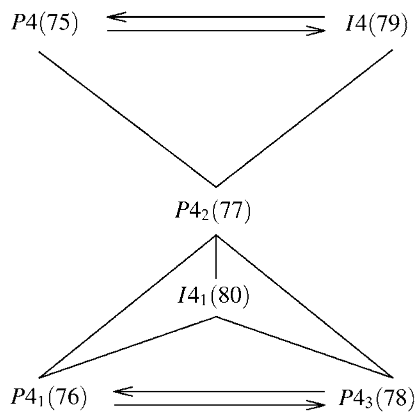

Fig. 2.5.2.1. Graph of the *klassengleiche* subgroups of the space groups of crystal class 4.

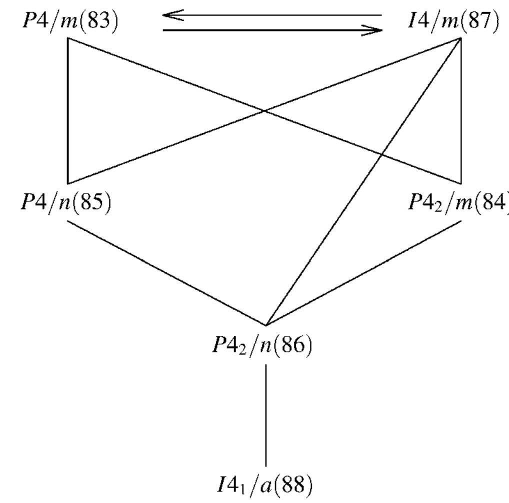

Fig. 2.5.2.3. Graph of the *klassengleiche* subgroups of the space groups of crystal class $4/m$.

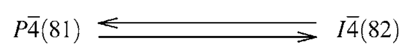

Fig. 2.5.2.2. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\overline{4}$.

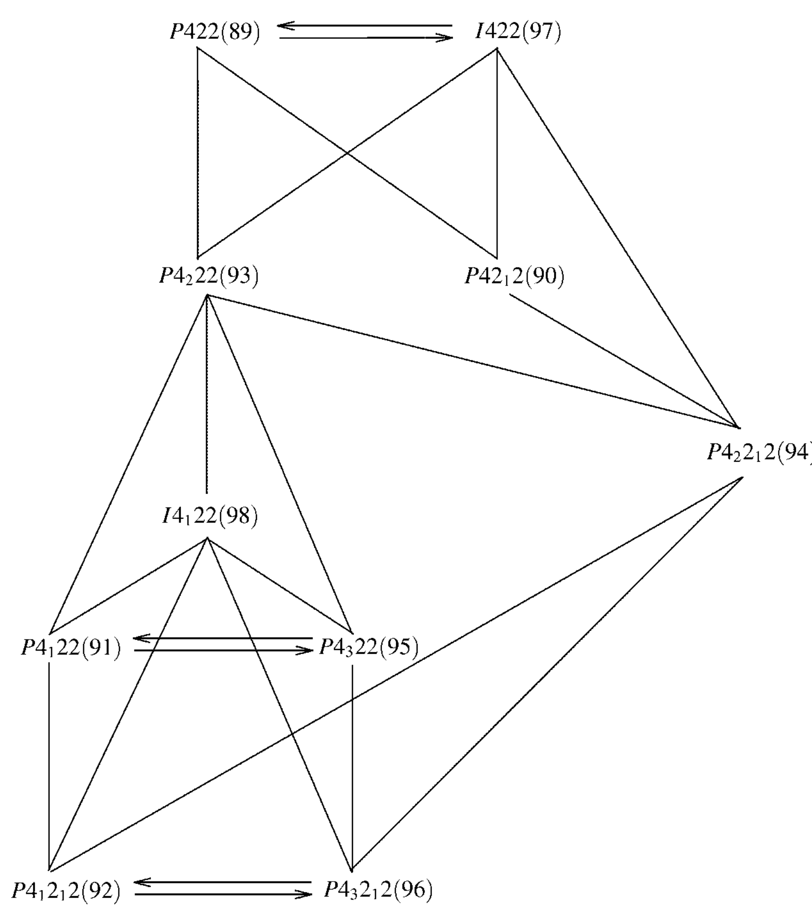

Fig. 2.5.2.4. Graph of the *klassengleiche* subgroups of the space groups of crystal class 422.

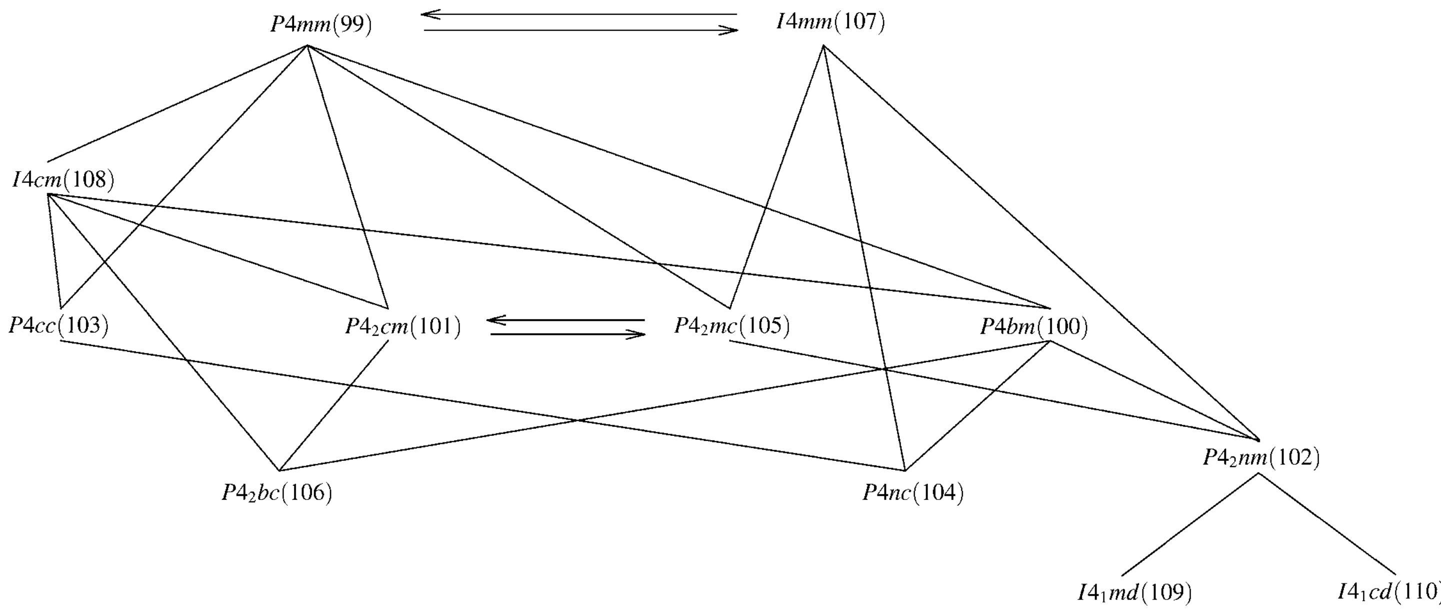

Fig. 2.5.2.5. Graph of the *klassengleiche* subgroups of the space groups of crystal class 4*mm*.

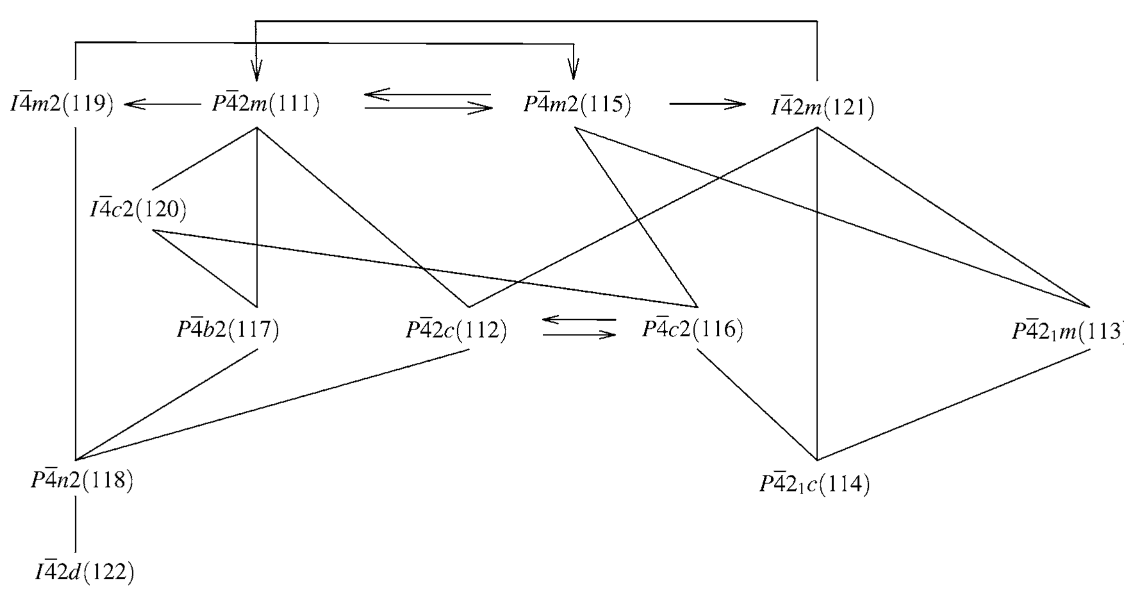

Fig. 2.5.2.6. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\bar{4}2m$.

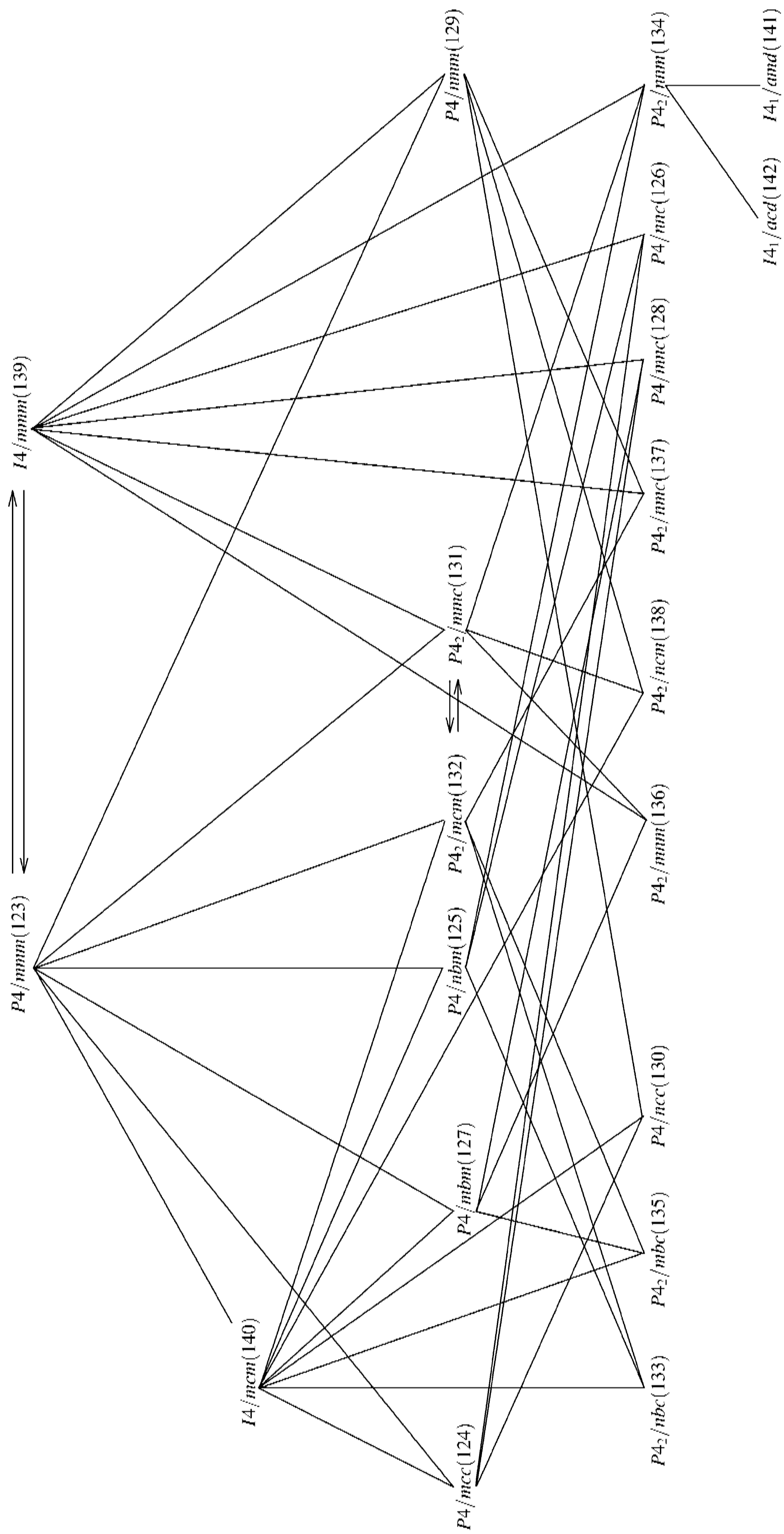

Fig. 2.5.2.7. Graph of the *klassengleiche* subgroups of the space groups of crystal class $4/mmm$.

2.5.3. Graphs of the *klassengleiche* subgroups of trigonal space groups

For an explanation of these graphs, see Section 2.1.7.3 (p. 55).

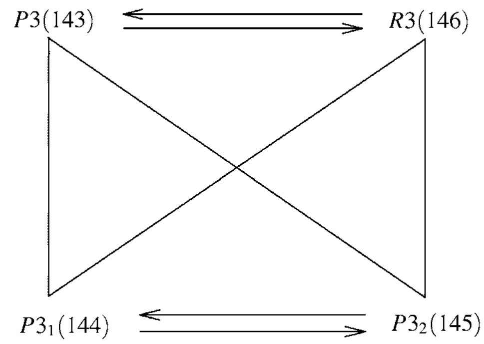

Fig. 2.5.3.1. Graph of the *klassengleiche* subgroups of the space groups of crystal class 3.

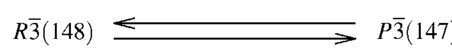

Fig. 2.5.3.2. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\bar{3}$.

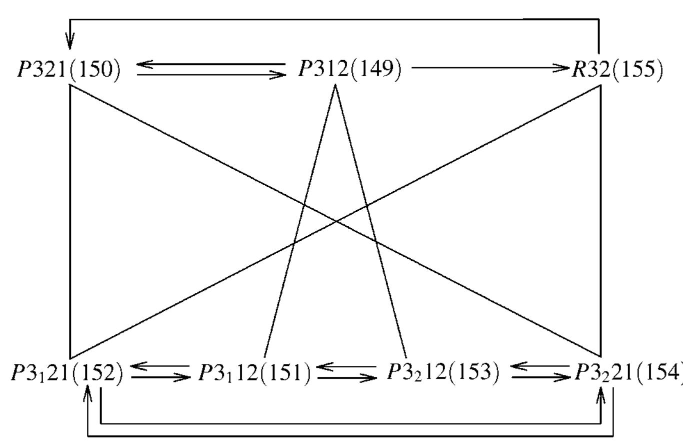

Fig. 2.5.3.3. Graph of the *klassengleiche* subgroups of the space groups of crystal class 32.

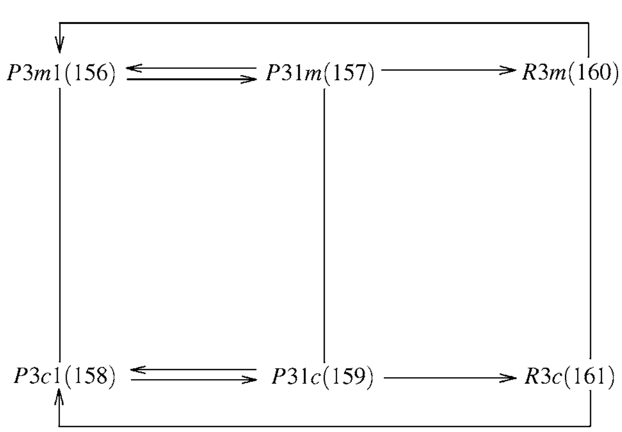

Fig. 2.5.3.4. Graph of the *klassengleiche* subgroups of the space groups of crystal class 3*m*.

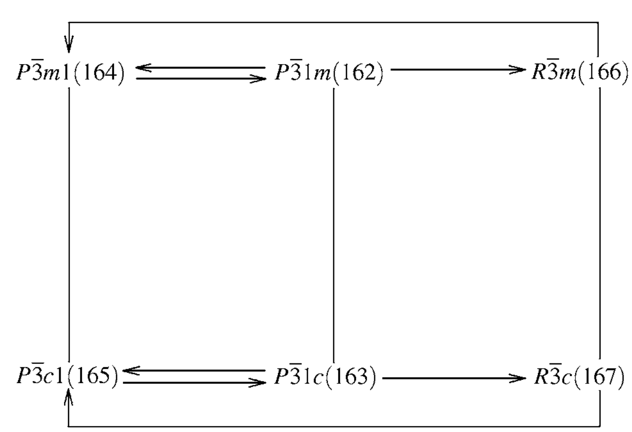

Fig. 2.5.3.5. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\bar{3}m$.

2.5.4. Graphs of the *klassengleiche* subgroups of hexagonal space groups

For an explanation of these graphs, see Section 2.1.7.3 (p. 55).

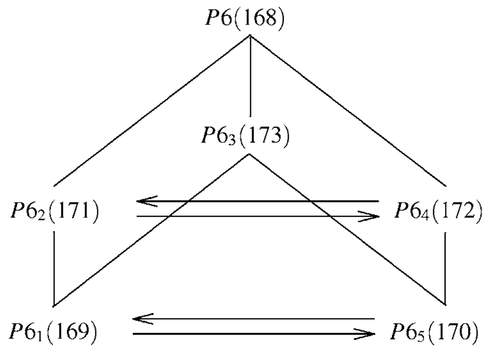

Fig. 2.5.4.1. Graph of the *klassengleiche* subgroups of the space groups of crystal class 6.

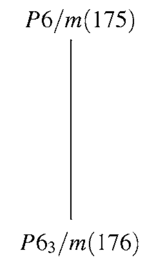

Fig. 2.5.4.2. Graph of the *klassengleiche* subgroups of the space groups of crystal class $6/m$.

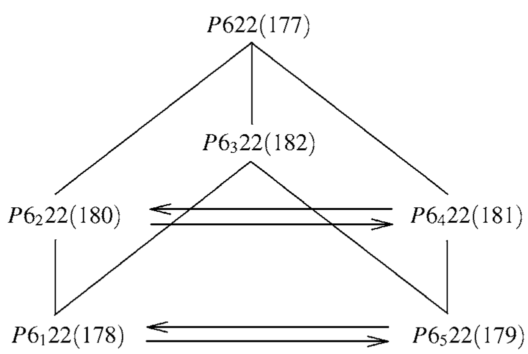

Fig. 2.5.4.3. Graph of the *klassengleiche* subgroups of the space groups of crystal class 622.

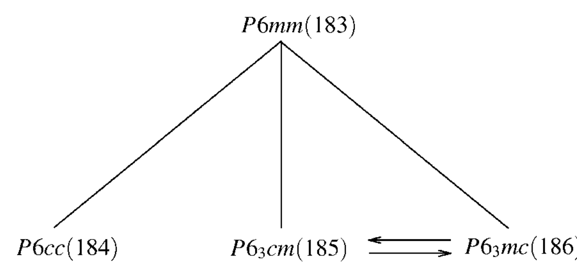

Fig. 2.5.4.4. Graph of the *klassengleiche* subgroups of the space groups of crystal class $6mm$.

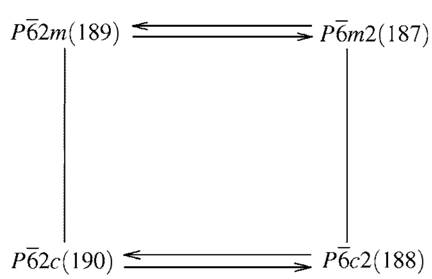

Fig. 2.5.4.5. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\bar{6}2m$.

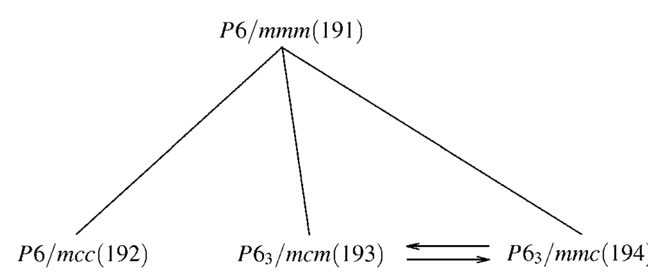

Fig. 2.5.4.6. Graph of the *klassengleiche* subgroups of the space groups of crystal class $6/mmm$.

2.5.5. Graphs of the *klassengleiche* subgroups of cubic space groups

For an explanation of these graphs, see Section 2.1.7.3 (p. 55).

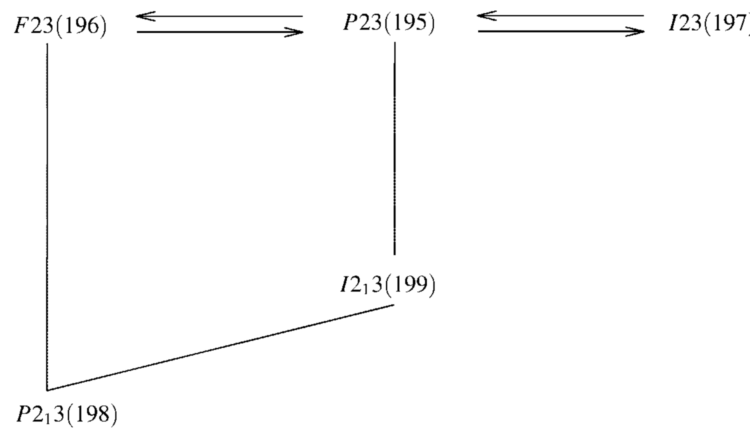

Fig. 2.5.5.1. Graph of the *klassengleiche* subgroups of the space groups of crystal class 23.

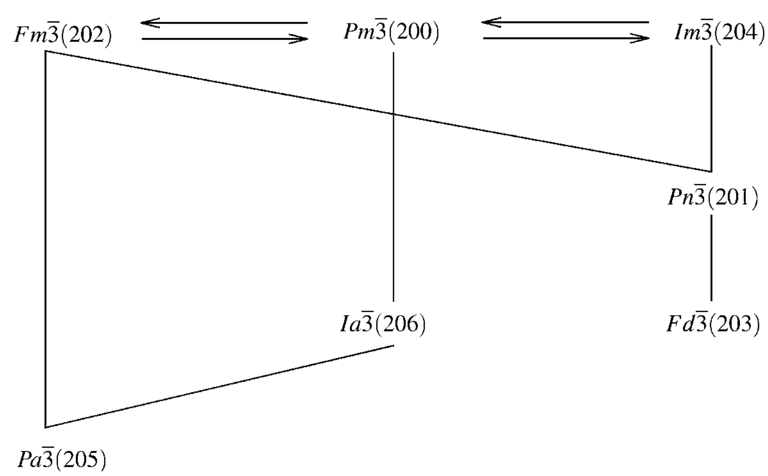

Fig. 2.5.5.2. Graph of the *klassengleiche* subgroups of the space groups of crystal class $m\overline{3}$.

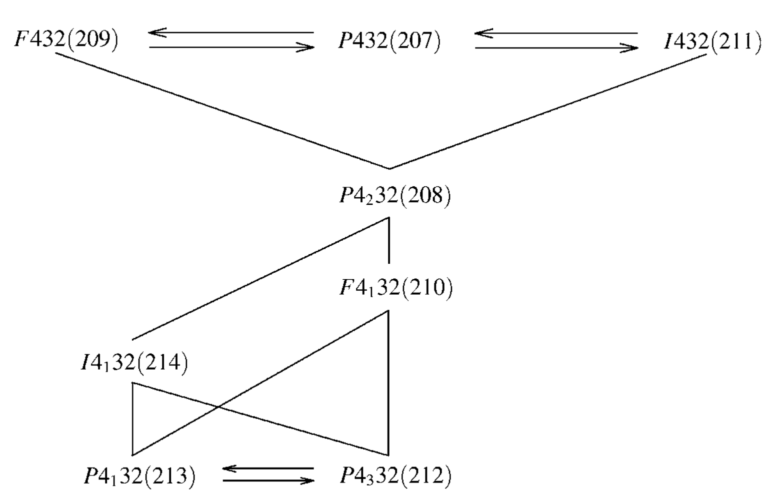

Fig. 2.5.5.3. Graph of the *klassengleiche* subgroups of the space groups of crystal class 432.

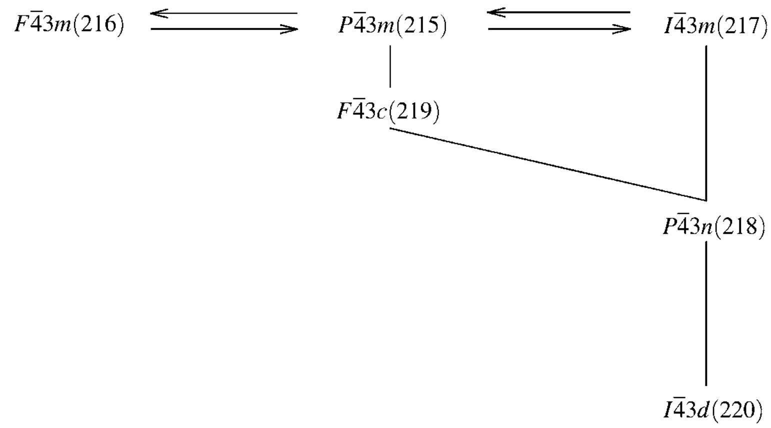

Fig. 2.5.5.4. Graph of the *klassengleiche* subgroups of the space groups of crystal class $\bar{4}3m$.

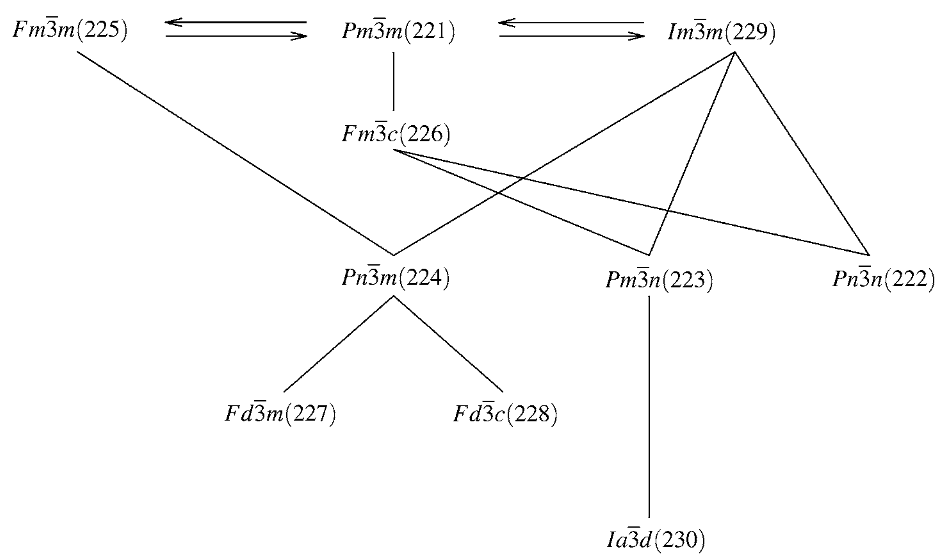

Fig. 2.5.5.5. Graph of the *klassengleiche* subgroups of the space groups of crystal class $m\bar{3}m$.

references

International Tables for Crystallography (2006). Vol. A1, Chapter 3.1, pp. 428–433.

3.1. Guide to the tables

BY ULRICH MÜLLER

In the tables of Chapter 3.2, all maximal subgroups of the space groups are listed. For all Wyckoff positions of a space group the relations to the Wyckoff positions of the subgroups are given. The Wyckoff positions are always labelled by their multiplicities and their Wyckoff letters, in the same manner as in *International Tables for Crystallography*, Volume A (2002). Reference to Volume A therefore is always necessary, especially when the corresponding coordinate triplets or site symmetries are needed. For general remarks on Wyckoff positions see Chapter 1.3.

3.1.1. Arrangement of the entries

Every space group begins on a new page (with the exception of $P4_3$, $P3_2$, $P6_4$ and $P6_5$, which are listed together with $P4_1$, $P3_1$, $P6_2$ and $P6_1$, respectively). If necessary, continuation occurs on the following page(s), or, in a few correspondingly marked cases, on the preceding page.

The different settings for monoclinic space groups are continued on the same or the following page(s).

3.1.1.1. *Headline*

The headline lists from the outer margin inwards:

(1) The *short Hermann–Mauguin symbol*;
(2) The number of the space group according to Volume A;
(3) The *full Hermann–Mauguin symbol* if it differs from the short symbol;
(4) The *Schoenflies symbol*.

In the case of monoclinic space groups, the headline can have one or two additional entries with the full Hermann–Mauguin symbols for different settings.

3.1.1.2. *Specification of the settings*

Each of the monoclinic space groups is listed several times, namely with unique axis b and with unique axis c, and, if applicable, with the three cell choices 1, 2 and 3 according to Volume A. Space permitting, the entries for the different settings have been combined on one page or on facing pages, since in most cases the Wyckoff-position relations do not depend on the choice of setting. In the few cases where there is a dependence, arrows ($\Rightarrow$) in the corresponding lines show to which settings they refer. Otherwise, the Wyckoff positions of the subgroups correspond to all of the settings listed on the same page or on facing pages.

The comment 'Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3' under a table refers to the infinite series of isomorphic subgroups listed at the bottom of a table of a monoclinic space group. For a given index p (p = prime number) and enlargement of the basis vectors perpendicular to the monoclinic axis, there are $p+1$ non-conjugate isomorphic maximal subgroups. Their cells can be calculated by formulae such as '$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$' and '$p\mathbf{a}$, $\mathbf{b}$, $q\mathbf{a}+\mathbf{c}$' with an integer parameter q taking any value from $-\frac{1}{2}(p-1)$ to $\frac{1}{2}(p-1)$. The same value of q may refer to a different subgroup for cell choices 1, 2 or 3.

Rhombohedral space groups are listed only in the setting with hexagonal axes with a rhombohedrally centred obverse cell [*i.e.* $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$]. However, for cubic space groups, the rhombohedral subgroups are also given with rhombohedral axes.

Settings with different origin choices are taken account of by two separate columns 'Coordinates' with the headings 'origin 1' and 'origin 2'.

3.1.1.3. *List of Wyckoff positions*

Under the column heading 'Wyckoff positions', the complete sequence of the Wyckoff positions of the space group is given by their multiplicities and Wyckoff letters. If necessary, the sequence runs over two or more lines.

3.1.1.4. *Subgroup data*

The subgroups are divided into two sections: **I Maximal *translationengleiche* subgroups** and **II Maximal *klassengleiche* subgroups**. The latter are further subdivided into three blocks:

Loss of centring translations. This block appears only if the space group has a conventionally centred lattice. The centring has been fully or partly lost in the subgroups listed. The size of the conventional unit cell is not changed.

Enlarged unit cell, non-isomorphic. The *klassengleiche* subgroups listed in this block are non-isomorphic and have conventional unit cells that are enlarged compared with the unit cell of the space group.

Enlarged unit cell, isomorphic. The listing includes the isomorphic subgroups with the smallest possible indices for every kind of cell enlargement. If they exist, index values of 2, 3 and 4 are always given (except for $P\bar{1}$, which is restricted to index 2). If the indices 2, 3 or 4 are not possible, the smallest possible index for the kind of cell enlargement considered is listed. In addition, the infinite series of isomorphic subgroups are given for all possible kinds of cell enlargements. The factor of the cell enlargement corresponds to the index, which is a prime number p, a square p^2 of a prime number, or a cube p^3 of a prime number (*cf.* Section 3.1.1.6). If $p > 2$, the specifically listed subgroups with small index values also always belong to the infinite series, so that the corresponding information is given twice in these cases. For $p = 2$ this applies only to certain special cases.

3.1.1.5. *Sequence of the listed subgroups*

Within each of the aforementioned blocks, the subgroups are listed in the following order. First priority is given to the index, with smallest values first. Subgroups with the same index follow decreasing space-group numbers (according to Volume A). Exception: the *translationengleiche* subgroup of a tetragonal space group listed last is always the one with the axes transformation to a diagonally oriented cell.

Translationengleiche subgroups of cubic space groups are in the order cubic, rhombohedral, tetragonal, orthorhombic.

In the case of the isomorphic subgroups, there is a subdivision according to the kind of cell enlargement. For monoclinic, tetragonal, trigonal and hexagonal space groups, cell enlargements in the direction of the unique axis are given first. For orthorhombic space groups, the isomorphic subgroups with increased **a** are given first, followed by increased **b** and **c**.

The sequence differs somewhat from that in Chapter 2.3 of this volume. In Chapter 2.3, the *klassengleiche* subgroups have been subdivided in more detail according to the different kinds of cell enlargements and the isomorphic subgroups with specific index values have been listed together with the *klassengleiche* subgroups, *i.e.* separately from the infinite series of isomorphic subgroups. A list of the differences in presentation between Chapters 2.3 and 3.2 is given in the Appendix at the end of this volume.

3.1.1.6. *Information for every subgroup*

3.1.1.6.1. *Index*

The entry for every subgroup begins with the index in brackets, for example [2] or [p] or [p^2] (p = prime number).

The index for any of the infinite number of maximal isomorphic subgroups must be either a prime number p, or, in certain cases of tetragonal, trigonal and hexagonal space groups, a square of a prime number p^2; for isomorphic subgroups of cubic space groups the index may only be the cube of a prime number p^3. In many instances only certain prime numbers are allowed (Bertaut & Billiet, 1979; Billiet & Bertaut, 2002; Müller & Brelle, 1995). If restrictions exist, the prime numbers allowed are given under the axes transformations by formulae such as '$p = \text{prime} = 3n - 1$'.

3.1.1.6.2. *Subgroup symbol*

The index is followed by the Hermann–Mauguin symbol (short symbol) and the space-group number of the subgroup. If a nonconventional setting has been chosen, then the space-group symbol of the conventional setting is also mentioned in the following line after the symbol $\widehat{=}$.

In some cases of nonconventional settings, the space-group symbol does not show uniquely in which manner it deviates from the conventional setting. For example, the nonconventional setting $P22_12$ of the space group $P222_1$ can result from cyclic exchange of the axes, $(\mathbf{b}, \mathbf{c}, \mathbf{a})$ or by interchange of $\mathbf{b}$ with $\mathbf{c}$ $(\mathbf{a}, -\mathbf{c}, \mathbf{b})$. As a consequence, the relations between the Wyckoff positions can be different. In such cases, cyclic exchange has always been chosen.

3.1.1.6.3. *Basis vectors*

The column 'Axes' shows how the basis vectors of the unit cell of a subgroup result from the basis vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ of the space group considered. This information is omitted if there is no change of basis vectors.

A formula such as '$q\mathbf{a} - r\mathbf{b}$, $r\mathbf{a} + q\mathbf{b}$, $\mathbf{c}$' together with the restrictions '$p = q^2 + r^2 = \text{prime} = 4n + 1$' and '$q = 2n + 1 \geq 1$; $r = \pm 2n' \neq 0$' means that for a given index p there exist several subgroups with different lattices depending on the values of the integer parameters q (odd) and r (even) within the limits of the restriction. In this example, the prime number p must be $p \equiv 1$ modulo 4 (*i.e.* 5, 13, 17, ...); if it is, say, $p = 13 = 3^2 + (\pm 2)^2$, the values of q and r may be $q = 3$, $r = 2$ and $q = 3$, $r = -2$.[1]

3.1.1.6.4. *Coordinates*

The column 'Coordinates' shows how the atomic coordinates of the subgroups are calculated from the coordinates x, y and z of the starting unit cell. This includes coordinate shifts whenever a shift of the origin is required (*cf.* Section 3.1.3). If the cell of the subgroup is enlarged, the coordinate triplet is followed by a semicolon; then follow fractional numbers in parentheses. This means that in addition to the coordinates given before the semicolon, further coordinates have to be considered; they result from adding the numbers in the parentheses. However, if the subgroup has a centring, the values to be added due to this centring are not mentioned. If no transformation of coordinates is necessary, the entry is omitted.

Example 3.1.1.6.1.

The entry

$$\tfrac{1}{3}x + \tfrac{1}{4}, y + \tfrac{1}{4}, z; \pm(\tfrac{1}{3}, 0, 0)$$

means: starting from the coordinates of, say, 0.63, 0.12, 0.0, sites with the following coordinates result in the subgroup:

0.46, 0.37, 0.0; 0.793333, 0.37, 0.0;
0.1266667, 0.37, 0.0.

Example 3.1.1.6.2.

The entry of an I-centred subgroup

$$\tfrac{1}{2}x, \tfrac{1}{2}y, \tfrac{1}{2}z; +(\tfrac{1}{2}, 0, 0); +(0, \tfrac{1}{2}, 0); +(0, 0, \tfrac{1}{2})$$

means: starting from the coordinates of, say, 0.08, 0.14, 0.20, sites with the following coordinates result in the subgroup:

0.04, 0.07, 0.10; 0.54, 0.07, 0.10;
0.04, 0.57, 0.10; 0.04, 0.07, 0.60;

in addition, there are all coordinates with $+(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})$ due to the I-centring:

0.54, 0.57, 0.60; 0.04, 0.57, 0.60;
0.54, 0.07, 0.60; 0.54, 0.57, 0.10.

For the infinite series of isomorphic subgroups, coordinate formulae are, for example, in the form $x, y, \tfrac{1}{p}z; +(0, 0, \tfrac{u}{p})$ with $u = 1, \ldots, p-1$. Then there are p coordinate values running from $x, y, \tfrac{1}{p}z$ to $x, y, \tfrac{1}{p}z + \tfrac{p-1}{p}$.

Example 3.1.1.6.3.

For a subgroup with index $p^2 = 25$ ($p = 5$) the entry

$$\tfrac{1}{p}x, \tfrac{1}{p}y, z; +(\tfrac{u}{p}, \tfrac{v}{p}, 0); u, v = 1, \ldots, p-1$$

means: starting from the coordinates of, say, 0.10, 0.35, 0.0, sites with the following coordinates result in the subgroup:

0.02, 0.07, 0.0; 0.02, 0.27, 0.0; 0.02, 0.47, 0.0;
0.02, 0.67, 0.0; 0.02, 0.87, 0.0;
0.22, 0.07, 0.0; 0.22, 0.27, 0.0; 0.22, 0.47, 0.0;
0.22, 0.67, 0.0; 0.22, 0.87, 0.0;
0.42, 0.07, 0.0; 0.42, 0.27, 0.0; 0.42, 0.47, 0.0;
0.42, 0.67, 0.0; 0.42, 0.87, 0.0;
0.62, 0.07, 0.0; 0.62, 0.27, 0.0; 0.62, 0.47, 0.0;
0.62, 0.67, 0.0; 0.62, 0.87, 0.0;
0.82, 0.07, 0.0; 0.82, 0.27, 0.0; 0.82, 0.47, 0.0;
0.82, 0.67, 0.0; 0.82, 0.87, 0.0.

If Volume A allows two choices for the origin, coordinate transformations for both are listed in separate columns with the headings 'origin 1' and 'origin 2'. If two origin choices are allowed for both the group as well as the subgroup, then it is understood that the origin choices of the group and the subgroup are the same (either origin choice 1 for both groups or origin choice 2 for both). If the space group has only one origin choice, but the subgroup

[1] If the sum of two square numbers is a prime number p, then it is $p = 2$ or $p = 4n + 1$, and every prime number of this type can be expressed as such a sum. Index number restrictions of this kind occur among isomorphic subgroups of certain tetragonal space groups. A similar relation occurring among trigonal and hexagonal space groups concerns prime numbers $p = q^2 - qr + r^2$; $p = 3$ or $p = 6n + 1$ always holds for integer q, r and every prime number $p = 6n + 1$ can be expressed by such a sum. For details, see Müller & Brelle (1995).

has two choices, the coordinate transformations are given for both choices on separate lines.

3.1.1.6.5. *Wyckoff positions*

The columns under the heading 'Wyckoff positions' contain the Wyckoff symbols of all sites of the subgroups that result therefrom. They are given in the same sequence as in the top line(s). If the symbols at the top run over more than one line, then the symbols for the subgroups take a corresponding number of lines.

When an orbit splits into several independent orbits, the corresponding Wyckoff symbols are separated by semicolons, *i.e.* $1b;4h;4k$. An entry such as $3 \times 8j$ means that a splitting into three orbits takes place, all of which are of the same kind $8j$; they differ in the values of their free parameters.

For the infinite series of isomorphic subgroups general formulae are given. They allow the calculation of the Wyckoff-position relations for any index in a simple manner.

Example 3.1.1.6.4.
The entry $\frac{p(p-1)}{2} \times 24k$ means that for a given prime number p, say $p = 5$, there are $\frac{5(5-1)}{2} = 10$ orbits of the kind $24k$.

In some cases of splittings, there is not enough space to enter all Wyckoff symbols on one line; this requires them to be listed one below the other over two or more lines. Whenever a Wyckoff symbol is followed by a semicolon, another symbol follows.

Example 3.1.1.6.5.
The last subgroup listed for space group $I\bar{4}m2$, No. 119, is $I\bar{4}m2$ with basis vectors $p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$. The entry for the Wyckoff position $2a$ is:

$$\left|\begin{array}{c} 2a; \frac{p-1}{2} \times 8g; \\ \frac{p-1}{2} \times 8i; \\ \frac{(p-1)(p-3)}{8} \times 16j \end{array}\right|$$

If $p = 5$, it shows the splitting of an orbit of position $2a$ into one orbit $2a$, two $(\frac{5-1}{2} = 2)$ orbits $8g$, two orbits $8i$ and one $(\frac{(5-1)(5-3)}{8} = 1)$ orbit $16j$.

Sometimes a Wyckoff label is followed by another Wyckoff label in parentheses together with a footnote marker. In this case, the Wyckoff label in parentheses is to be taken for the cases specified in the footnote.

Example 3.1.1.6.6.
The entry $2c(d^*)$ together with the footnote $^*\, p = 4n-1$ means that the Wyckoff position is $2c$, but it is $2d$ if the index is $p \equiv 3$ modulo 4 (*i.e.* $p = 3, 7, 11, \ldots$).

The Wyckoff positions of an isomorphic subgroup of a space group with two choices for the origin are only identical for the two choices if certain origin shifts are taken into account. Since origin shifts have been avoided as far as possible, in some cases some Wyckoff positions differ for the two origin choices.

Example 3.1.1.6.7.
The isomorphic subgroups of the space group $P4_2/n$, No. 86, with cell enlargements $\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$ and $p = 4n - 1$ result in identical Wyckoff positions for the two origin choices only if there is no origin shift for choice 1, but an origin shift of $0, 0, \frac{1}{2}$ for choice 2. The origin shift for choice 2 has been avoided, but as a consequence some of the Wyckoff labels differ for the two choices. For the Wyckoff position $2a$ of the space group, the entry for these isomorphic subgroups is $2a(b^\dagger); \frac{p-1}{2} \times 4f$. The footnote reads '† origin 2 and $p = 4n - 1$'. Therefore, $2a$ is (aside from $4f$) the resulting Wyckoff position for origin choice 1 and any value of p; for origin choice 2 it is also $2a$ if $p = 4n + 1$, but it is $2b$ if $p = 4n - 1$ (the permitted values for p are $p = 4n \pm 1$).

Warning: *The listed Wyckoff positions of the subgroups apply only to the transformations given in the column 'Coordinates'.* If other cell transformations or origin shifts are used, this may result in an interchange of Wyckoff positions within each Wyckoff set of the subgroup.

3.1.2. Cell transformations

When comparing related crystal structures, unit-cell transformations are troublesome. They result in differing sets of atomic coordinates for corresponding atoms; this can make comparisons more complicated and structural relations may be obscured. Frequently, it is more convenient not to interchange axes and to avoid transformations if possible. The use of a nonconventional setting of a space group may be preferable if this reduces cell transformations. For this reason, in the present tables settings of the subgroups were preferentially chosen in such a way that the directions of the basis vectors of a space group and its subgroup deviate as little as possible. If this results in a nonconventional setting of the subgroup, then the way to transform the basis vectors and coordinates to those of the conventional cell is also given.

Subgroups listed in nonconventional settings concern orthorhombic and monoclinic space groups. Their transformations to conventional settings frequently only involve an interchange of axes. In the case of tetragonal subgroups, nonconventional settings with C-centred or F-centred cells are not used; this would have caused nonconventional multiplicities of the Wyckoff positions and would have required listings of all positions in these settings. Equally, face-centred monoclinic cells, B-centred monoclinic cells for unique axis b, C-centred monoclinic cells for unique axis c and hexagonal H cells are not used.

Monoclinic space groups allow different descriptions, such as unique axis a, b or c, base- or body-centred cells, and glide vectors in different directions. All settings that are listed in Volume A have been considered to be allowed conventional settings. Whenever a cell transformation can be avoided and the subgroup conforms to any of the settings listed in Volume A (b or c as unique axis; cell choices 1, 2 or 3), then this setting has been chosen. Transformations to other settings are not given in these cases.

3.1.3. Origin shifts

In a group–subgroup relation, an origin shift may be necessary to conform to the conventional origin setting of the subgroup. This causes coordinate changes for equivalent atomic positions and is therefore undesirable for the purpose of comparing related crystal structures. However, in some cases an origin shift can be avoided if the relations between the basis vectors are chosen in a convenient manner. For example, the isomorphic relation of index 27 (for short: $i27$)

$$F4_132 \xrightarrow{i27} F4_132$$

requires an increase of the lattice parameters by a factor of 3. To conform to the conventional setting, the origin must by displaced when the cell of the subgroup is chosen to be $3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$. However, no displacement is necessary when the cell of the subgroup is taken to be $3\mathbf{b}, -3\mathbf{a}, 3\mathbf{c}$. Although the x and $-y$ coordinates exchange places, this may be more convenient, since no values for an origin shift have to be added. For this reason, the latter option is preferred in this case.

Origin shifts can be specified in terms of the coordinate system of the starting space group or of the coordinate system of the subgroup. In Part 2 of this volume, all origin shifts refer to the starting space group. In Part 3, the origin shifts are contained in the column 'Coordinates' as additive fractional numbers. This means that these shifts refer to the *coordinate system of the subgroup*.

When comparing related crystal structures, it is mainly the atomic coordinates which have to be interconverted. Thus the coordinate conversion formulae are needed anyway; they are given in the column 'Coordinates'. When space groups are involved that allow two origin choices, the origin shifts from a group to a subgroup can be different depending on whether origin choice 1 or 2 has been selected. Therefore, all space groups with two origin choices have two columns 'Coordinates', one for each origin choice. The coordinate conversion formulae for a specific subgroup in the two columns only differ in the additive fractional numbers that specify the origin shift. In addition, origin shifts could also have been specified in terms of the coordinate system of the starting space group. This, however, would have been redundant information that would have required an additional column, causing a serious shortage of space.

The origin shifts listed in the column 'Coordinates' can be converted to origin shifts that refer to the coordinate system of the starting space group in the following way:

Take:

$\mathbf{a}, \mathbf{b}, \mathbf{c}$	basis vectors of the starting space group;
O	origin of the starting space group;
$\mathbf{a}', \mathbf{b}', \mathbf{c}'$	basis vectors of the subgroup;
O'	origin of the subgroup;
$x_{o'}, y_{o'}, z_{o'}$	coordinates of O' expressed in the coordinate system of the starting group;
x'_o, y'_o, z'_o	coordinates of O expressed in the coordinate system of the subgroup.

The basis vectors are related according to

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}.$$

$\boldsymbol{P}$ is the 3×3 transformation matrix of the basis change. The origin shift $O \to O'$ then corresponds to the vector

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\boldsymbol{P} \begin{pmatrix} x'_o \\ y'_o \\ z'_o \end{pmatrix}.$$

Example 3.1.3.1.

In the group–subgroup relation $Fddd \to C12/c1$, a cell transformation and an origin shift are needed if origin choice 1 has been selected for $Fddd$. In the table for space group $Fddd$, No. 70, the transformation of the basis vectors in the column 'Axes' is given as $\mathbf{a}$, $-\mathbf{b}$, $-\frac{1}{2}(\mathbf{a}+\mathbf{c})$, which means that the transformation matrix is

$$\boldsymbol{P} = \begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix}.$$

In the column 'Coordinates' for origin choice 1, the coordinate transformations are given as x–z, $-y+\frac{1}{8}$, $-2z+\frac{1}{4}$, which implies a coordinate shift of $x'_o = 0$, $y'_o = \frac{1}{8}$ and $z'_o = \frac{1}{4}$ referred to the coordinate system of the subgroup $C12/c1$, No. 15. The origin shift in terms of the starting space group $Fddd$ is

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{8} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{8} \\ \frac{1}{8} \\ \frac{1}{8} \end{pmatrix}.$$

Example 3.1.3.2.

Consider space group $Pnma$, No. 62, and its subgroup $P2_12_12_1$, No. 19. In the table for space group $Pnma$, the coordinate transformation in the column 'Coordinates' is given as $x, y, z+\frac{1}{4}$. Therefore, there is no basis transformation, $\boldsymbol{P} = \boldsymbol{I}$, but there is an origin shift of $x'_o = 0$, $y'_o = 0$, $z'_o = \frac{1}{4}$ expressed in the coordinate system of $P2_12_12_1$. In terms of the coordinate system of $Pnma$ this coordinate shift has the opposite sign:

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -\frac{1}{4} \end{pmatrix}.$$

Note: In Chapter 2.3, the listed origin shifts refer to the starting space group and thus are given in a different way to that in Chapter 3.2. In addition, for a given group–subgroup pair the direction of the origin shift selected in Chapter 2.3 usually differs from the origin shift listed in Chapter 3.2 (often the direction is opposite; see the Appendix).

3.1.4. Nonconventional settings of orthorhombic space groups

Orthorhombic space groups can have as many as six different settings, as listed in Chapter 4.3 of Volume A. They result from the interchange of the axes **a**, **b**, **c** in the following ways:

Cyclic exchange: **bca** or **cab**.

Exchange of two axes, combined with the reversal of the direction of one axis in order to keep a right-handed coordinate system:

$\mathbf{b}\mathbf{a}\bar{\mathbf{c}}$ or $\mathbf{b}\bar{\mathbf{a}}\mathbf{c}$ or $\bar{\mathbf{b}}\mathbf{a}\mathbf{c}$;
$\mathbf{c}\mathbf{b}\bar{\mathbf{a}}$ or $\mathbf{c}\bar{\mathbf{b}}\mathbf{a}$ or $\bar{\mathbf{c}}\mathbf{b}\mathbf{a}$;
$\mathbf{a}\mathbf{c}\bar{\mathbf{b}}$ or $\mathbf{a}\bar{\mathbf{c}}\mathbf{b}$ or $\bar{\mathbf{a}}\mathbf{c}\mathbf{b}$.

The exchange has two consequences for a Hermann–Mauguin symbol:

(1) the symmetry operations given in the symbol interchange their positions in the symbol;
(2) the labels of the glide directions and of the centrings are interchanged.

In the same way, the sequences and the labels and values of the coordinate triplets have to be interchanged.

Example 3.1.4.1.

Take space group $Pbcm$, No. 57 (full symbol $P2/b2_1/c2_1/m$), and its Wyckoff position $4c$ $(x, \frac{1}{4}, 0)$. The positions in the symbol change as given by the arrows, and simultaneously the labels change:

abc: $P2/b2_1/c2_1/m$	$x, \frac{1}{4}, 0$	**abc**: $P2/b2_1/c2_1/m$ $x, \frac{1}{4}, 0$
bca: $P2_1/b2_1/m2/a$	$\frac{1}{4}, 0, z$	$\mathbf{b}\bar{\mathbf{a}}\mathbf{c}$: $P2_1/c\,2/a\,2_1/m$ $\frac{1}{4}, -y, 0$

The notation **bca** means: the former b axis is now in the position of the a axis *etc.* or: convert b to a, c to b, and a to c.

The corresponding interchanges of positions and labels for all possible nonconventional settings are listed at the end of the table of each orthorhombic space group. They have to be applied to all subgroups.

Example 3.1.4.2.

Consider the nonconventional setting *Pcam* of *Pbcm*. The entry at the bottom of the page for space group *Pbcm*, No. 57, shows the necessary interchanges for the setting *Pcam*: $a \rightleftarrows b$, $\mathbf{a} \rightleftarrows -\mathbf{b}$, and $x \rightleftarrows -y$.

For the subgroup *Pbna* (last entry in the block of *klassengleiche* non-isomorphic subgroups) this means: *Pbna* has to be replaced by *Pnab*, the axes conversion $2\mathbf{a}, \mathbf{b}, \mathbf{c}$ has to be replaced by $\mathbf{a}, -2\mathbf{b}, \mathbf{c}$ and the coordinate transformation $\frac{1}{2}x + \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$ has to be replaced by $x, -\frac{1}{2}y - \frac{1}{4}, z; +(0, -\frac{1}{2}, 0)$.

Pbna and *Pnab* are nonconventional settings of *Pbcn*, No. 60.

The interchange of the axes does not affect the Wyckoff labels, just the corresponding coordinates.

Example 3.1.4.3.

The Wyckoff position $4c$ $(x, \frac{1}{4}, 0)$ of *Pbcm*, No. 57, retains its label for any of the other settings of this space group. In the setting *Pbma*, this Wyckoff position is still $4c$ and has the coordinates $\frac{1}{4}, 0, z$. In this case, no ambiguity arises because the different settings of space group *Pbcm* all have different Hermann–Mauguin symbols that uniquely show how the axes have to be interchanged (*Pmca*, *Pbma*, *Pcam*, *Pmab* and *Pcmb*).

The interchange of the axes must also be performed for those subgroups that have equivalent directions and where the Hermann–Mauguin symbol does not uniquely show the kind of setting. Otherwise, the wrong Wyckoff positions can result.

Example 3.1.4.4.

Space group *Cmmm*, No. 65, has two *klassengleiche* subgroups of type *Immm*, No. 71, with doubled c axis. In the nonconventional setting *Bmmm* of *Cmmm*, the same subgroups *Immm* result from a doubling of the b axis. In the conventional setting of *Immm*, the Wyckoff positions $4e$, $4g$ and $4i$ represent orbits with the coordinates $(x, 0, 0)$, $(0, y, 0)$ and $(0, 0, z)$, respectively. In the space group *Cmmm*, the position $4k$ corresponds to $(0, 0, z)$ and upon transition to either of the subgroups *Immm* it splits to $2 \times 4i$.

If *Bmmm* is obtained from *Cmmm* by cyclic exchange of the axes ($\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$), its Wyckoff position $4k$ obtains the coordinates $(0, y, 0)$. Upon doubling of b and transition to *Immm*, $4k$ will split to two orbits with the coordinates $(0, \frac{1}{2}y, 0)$ and $(0, \frac{1}{2}y + \frac{1}{2}, 0)$. These are two orbits $4i$ of *Immm*, but this is only correct if the axes of *Immm* have also been interchanged in the same way. *If the interchange of axes has not been performed in the subgroup Immm in the assumption that in Immm all axes are equivalent anyway, wrong results will be obtained*. That is, *Immm* also has to be used in a nonconventional setting, although this is not apparent from the Hermann–Mauguin symbol. Of course, the Wyckoff symbols can then be relabelled so that they correspond to the conventional listings of Volume A ($4i \rightarrow 4g$ *etc.*). It is recommended that this return to the conventional setting of *Immm* is performed, because using the label $4i$ for $(0, y, 0)$ in *Immm* is likely to cause confusion if the nonconventional setting is not explicitly stressed.

3.1.5. Conjugate subgroups

Conjugate subgroups are different subgroups belonging to the same space-group type (they have the same Hermann–Mauguin symbol) and they have the same unit-cell size and the same shape for the conventional cell. They can be mapped onto one another by a symmetry operation of the starting group, *i.e.* they are symmetry-equivalent in this space group. They can occur only if the index of symmetry reduction is ≥ 3. The relations of the Wyckoff positions of a space group with the Wyckoff positions of any representative of a set of conjugate subgroups are always the same. Therefore, in principle it is sufficient to list the relations for only one representative.

Two kinds of conjugation of maximal subgroups can be distinguished, translational conjugation and orientational conjugation. Non-maximal subgroups can involve both kinds of conjugation, so the situation is more complicated in chains of group–subgroup relations, *cf.* Koch (1984) and Müller (1992). Since the present tables only list maximal subgroups, we will not discuss this here.

3.1.5.1. *Translational conjugation*

Translational conjugation occurs when the group–subgroup relation involves a loss of translational symmetry. This happens when the conventional cell has been enlarged or when centring translations have been lost; this means that the primitive unit cell of the subgroup is larger (by a factor ≥ 3). Translationally conjugate subgroups of a space group are symmetry-equivalent by a translation of the lattice of this space group. This way, isomorphic subgroups of index $p \geq 3$ have p conjugate subgroups (unless the cell enlargement occurs in a direction in which the origin may float). The existence of conjugate subgroups of this kind is not specifically mentioned in the tables. However, they can be recognized by looking in the column 'Coordinates'. If a semicolon appears after the coordinate triplet, followed by values in parentheses to be added, and if, in addition, the index of symmetry reduction is ≥ 3, then conjugate subgroups usually exist. They differ in the locations of their origins by values corresponding to the values given in the parentheses.

Example 3.1.5.1.1.

$$x, y, \tfrac{1}{3}z;\ \pm(0, 0, \tfrac{1}{3})$$

gives the positional coordinates in the subgroup originating from the coordinates of one unit cell of the starting group, namely

$$x, y, \tfrac{1}{3}z; \quad x, y, \tfrac{1}{3}z + \tfrac{1}{3}; \quad x, y, \tfrac{1}{3}z - \tfrac{1}{3}.$$

In addition, this also means that there are three conjugate subgroups. They differ in the locations of their origins referred to the origin of the starting space group by $0, 0, 0$, $0, 0, \frac{1}{3}$ and $0, 0, -\frac{1}{3}$, expressed in terms of the coordinate system of the subgroup, which is equivalent to $0, 0, 0$, $0, 0, -1$ and $0, 0, 1$ in the coordinate system of the starting group.

Primitive subgroups of face-centred cubic space groups have four conjugate subgroups. Because in this case no values have to be added to the coordinates, the existence of conjugate subgroups is expressed by the entry '4 conjugate subgroups'. They differ in their origin locations corresponding to the centring vectors of the face-centred cell.

Cell enlargements do not always produce conjugate subgroups. If the cell is being enlarged in a direction in which the origin may float, *i.e.* is not fixed by symmetry, no conjugate subgroups result. This applies to the following crystal classes:

1, enlargement in any direction;

2, $mm2$, 3, $3m$, 4, $4mm$, 6 and $6mm$, enlargement in the direction of the unique axis;

m, enlargement parallel to the plane of symmetry.

Example 3.1.5.1.2.

The cell enlargement **a**, **b**, 5**c** of space group $Cmc2_1$, No. 36, (crystal class $mm2$) does not produce conjugate subgroups.

If one is unsure whether conjugate subgroups exist, this can be looked up in the tables of Chapter 2.3 of this volume, where all conjugate subgroups are always mentioned and joined by a left brace.

Example 3.1.5.1.3.

For space group $Pm\overline{3}m$, No. 221, two subgroups $Im\overline{3}m$ ($2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$) with index 4 are listed. Each of them belongs to a set of four conjugate subgroups which differ in their origin locations ($0,0,0; -1,0,0; 0,-1,0; 0,0,-1$ for the first listed subgroup, referred to the coordinate system of $Pm\overline{3}m$). This can be seen by the coordinate values to be added ($0,0,0; \frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$; coordinate system of $Im\overline{3}m$). In Chapter 2.3, all four conjugate subgroups and their origin shifts are listed and joined by a brace.

3.1.5.2. *Orientational conjugation*

In this case, the conjugate subgroups have differently oriented unit cells that are equivalent by a symmetry operation other than a translation of the space group. This occurs in the following cases: orthorhombic subgroups of hexagonal space groups; monoclinic subgroups of trigonal (including rhombohedral) space groups; rhombohedral and tetragonal subgroups of cubic space groups. In these cases, the corresponding cell and coordinate transformations are listed for all conjugate subgroups after the word ‘conjugate’. Their Wyckoff symbols, being the same for all conjugate subgroups, are not repeated.

Example 3.1.5.2.1.

The cubic space group $P\overline{4}3m$, No. 215, has three tetragonal conjugate subgroups $P\overline{4}2m$. Their tetragonal c axes correspond to the cubic a, b or c axes, respectively. In $P\overline{4}3m$, a, b and c are symmetry-equivalent by the threefold rotation axes.

3.1.6. Monoclinic and triclinic subgroups

Aside from the two choices for the unique axis and the three possible cell choices given in Volume A, the unit cell of a monoclinic space group allows many more settings that can be interconverted by transformations such as $\mathbf{a} \pm q\mathbf{c}, \mathbf{b}, \mathbf{c}$ with an integer value for q (Sayari & Billiet, 1977). The most commonly chosen cell is the one with the shortest basis vectors **a** and **c** and a non-acute angle β. For triclinic space groups the ‘reduced’ cell is preferred, which depends on the metric values of the lattice (Billiet & Rolley Le Coz, 1980).

Some relations always require a cell transformation, for example rhombohedral to monoclinic relations. A group–subgroup relation in which the subgroup is monoclinic or triclinic can always be chosen together with a cell transformation that produces one of the cells mentioned. The transformation to be chosen depends on the cell metrics of the starting space group. For general tables we therefore cannot specify *a priori* the kind of cell transformation that will be needed.

The settings listed for monoclinic and triclinic subgroups were chosen in such a way that axes transformations are avoided or kept to a minimum. Depending on the cell metrics, this may result in cells that do not have the shortest possible basis vectors. Unfortunately, transformation of a monoclinic or triclinic cell setting to another one may cause an interchange of Wyckoff labels (within the Wyckoff sets). Frequently, several possible cell settings of the same monoclinic subgroup have been listed; the entry for the subgroup then is followed by the word ‘or’ or ‘alternative’, plus another entry.

Example 3.1.6.1.

Space group $Cmcm$, No. 63, has the subgroup $P112_1/m$, No. 11. It requires a cell transformation which is given as $\mathbf{a}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}), \mathbf{c}$. The following two lines list two other possible cell transformations for the *same* subgroup after the words ‘or’: $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$ and $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$. These three options cause different relations for the Wyckoff positions $4b$ and $8d$ of $Cmcm$.

Caution should also be exerted when different cell choices of monoclinic cells are involved. Monoclinic subgroups may refer to any of the three cell choices listed in Volume A. As long as these cell choices are used as listed in Volume A, no problems should arise. However, interconversions from one setting to another and especially nonconventional settings require special attention.

Example 3.1.6.2.

The common setting of space group No. 15 is $C12/c1$, which means unique axis b and cell choice 1; the glide plane c is located at $y = 0$ (and $y = \frac{1}{2}$). By interchanging the axes **b** and $-\mathbf{c}$, $C12/c1$ becomes $B112/b$ with the b glide plane at $z = 0$. This was the setting listed in *International Tables for X-ray Crystallography* (1952, 1965, 1969) for unique axis c. However, since the 1983 edition of Volume A, $B112/b$ does not correspond to one of the listed cell choices. Instead, they are now $A112/a$ (cell choice 1) or $B112/n$ (cell choice 2) or $I112/b$ (cell choice 3). Note that for all three cell choices the glide plane mentioned in the symbol is at $z = 0$. $B112/n$ also has a glide plane in the **b** direction, but unlike $B112/b$ it is at $z = \frac{1}{4}$. $B112/n$ and $B112/b$ can be set up with the same unit-cell dimensions, but with origins shifted by $\frac{1}{4},0,\frac{1}{4}$. The full Hermann–Mauguin symbol always shows uniquely which is the setting.

$P1$ No. 1 C_1^1

Axes	Coordinates	Wyckoff positions
		$1a$

II Maximal *klassengleiche* subgroups

Enlarged unit cell, isomorphic

	Axes	Coordinates	$1a$
[2] $P1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$2\times 1a$
[2] $P1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$	$2\times 1a$
[2] $P1$	$\mathbf{a}, \mathbf{b}-\mathbf{c}, \mathbf{b}+\mathbf{c}$	$x, \frac{1}{2}(y-z), \frac{1}{2}(y+z);\ +(0, \frac{1}{2}, \frac{1}{2})$	$2\times 1a$
[2] $P1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, \frac{1}{2}(x+z);\ +(\frac{1}{2}, 0, \frac{1}{2})$	$2\times 1a$
[2] $P1$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z;\ +(\frac{1}{2}, \frac{1}{2}, 0)$	$2\times 1a$
[2] $P1$	$\mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+y-z), \frac{1}{2}(-x+y+z), \frac{1}{2}(x-y+z);\ +(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\times 1a$
[2] $P1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ (0, 0, \frac{1}{2})$	$2\times 1a$
[3] $P1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ +(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x-y), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+y+z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+y-z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-y+z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-y-z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 1a$
[3] $P1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	$3\times 1a$
[3] $P1$	$\mathbf{a}, 3\mathbf{b}, -\mathbf{b}+\mathbf{c}$	$x, \frac{1}{3}(y+z), z;\ \pm(0, \frac{1}{3}, 0)$	$3\times 1a$
[3] $P1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{b}+\mathbf{c}$	$x, \frac{1}{3}(y-z), z;\ \pm(0, \frac{1}{3}, 0)$	$3\times 1a$
[3] $P1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ (0, 0, \frac{1}{3})$	$3\times 1a$
[p] $P1$	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, r\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qy-rz), y, z;\ +(\frac{u}{p}, 0, 0)$	$p\times 1a$
	$p = \text{prime} > 2;\ u = 1, \dots p-1;$	$-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$ $-\frac{1}{2}(p-1) \le r \le \frac{1}{2}(p-1)$	
[p] $P1$	$\mathbf{a}, p\mathbf{b}, q\mathbf{b}+\mathbf{c}$	$x, \frac{1}{p}(y-qz), z;\ +(0, \frac{u}{p}, 0)$	$p\times 1a$
	$p = \text{prime} > 2;\ u = 1, \dots p-1;$	$-\frac{1}{2}(p-1), \le q \le \frac{1}{2}(p-1)$	
[p] $P1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0, 0, \frac{u}{p})$	$p\times 1a$
	$p = \text{prime};\ u = 1, \dots p-1;$		

C_i^1 No. 2 $P\bar{1}$

	Axes	Coordinates	Wyckoff positions				
			$1a$	$1b$ $1f$	$1c$ $1g$	$1d$ $1h$	$1e$ $2i$
I Maximal *translationengleiche* subgroups							
[2] $P1$ (1)			$1a$	$1a$ $1a$	$1a$ $1a$	$1a$ $1a$	$1a$ $2\times 1a$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[2] $P\bar{1}$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$	$1a; 1d$	$1b; 1f$ $2i$	$1c; 1e$ $1g; 1h$	$2i$ $2i$	$2i$ $2\times 2i$
[2] $P\bar{1}$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	$2i$	$2i$ $1b; 1f$	$2i$ $2i$	$1a; 1d$ $1g; 1h$	$1c; 1e$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}, \mathbf{b}+\mathbf{c}, -\mathbf{b}+\mathbf{c}$	$x, \frac{1}{2}(y+z), \frac{1}{2}(-y+z);$ $+(0, \frac{1}{2}, \frac{1}{2})$	$1a; 1g$	$2i$ $2i$	$2i$ $1b; 1c$	$1d; 1h$ $1e; 1f$	$2i$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}, \mathbf{b}+\mathbf{c}, -\mathbf{b}+\mathbf{c}$	$x, \frac{1}{2}(y+z)+\frac{1}{4}, \frac{1}{2}(-y+z)+\frac{1}{4};$ $+(0, \frac{1}{2}, \frac{1}{2})$	$2i$	$1a; 1g$ $1d; 1h$	$1b; 1c$ $2i$	$2i$ $2i$	$1e; 1f$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, \frac{1}{2}(x+z);$ $+(\frac{1}{2}, 0, \frac{1}{2})$	$1a; 1f$	$2i$ $1b; 1d$	$1c; 1h$ $2i$	$2i$ $1e; 1g$	$2i$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z)+\frac{1}{4}, y, \frac{1}{2}(x+z)+\frac{1}{4};$ $+(\frac{1}{2}, 0, \frac{1}{2})$	$2i$	$1b; 1d$ $2i$	$2i$ $1e; 1g$	$1a; 1f$ $2i$	$1c; 1h$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z;$ $+(\frac{1}{2}, \frac{1}{2}, 0)$	$1a; 1e$	$1b; 1h$ $2i$	$2i$ $2i$	$2i$ $1f; 1g$	$1c; 1d$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}(-x+y)+\frac{1}{4}, z;$ $+(\frac{1}{2}, \frac{1}{2}, 0)$	$2i$	$2i$ $1f; 1g$	$1a; 1e$ $1b; 1h$	$1c; 1d$ $2i$	$2i$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+y-z), \frac{1}{2}(-x+y+z),$ $\frac{1}{2}(x-y+z); +(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$1a; 1h$	$2i$ $1b; 1e$	$2i$ $1c; 1f$	$2i$ $2i$	$1d; 1g$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}+\mathbf{b}, \mathbf{b}+\mathbf{c}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+y-z)+\frac{1}{4}, \frac{1}{2}(-x+y+z)+\frac{1}{4},$ $\frac{1}{2}(x-y+z)+\frac{1}{4}; +(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2i$	$1d; 1g$ $2i$	$1b; 1e$ $2i$	$1c; 1f$ $1a; 1h$	$2i$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$	$1a; 1c$	$1b; 1g$ $1f; 1h$	$2i$ $2i$	$1d; 1e$ $2i$	$2i$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$	$2i$	$2i$ $2i$	$1a; 1c$ $1b; 1g$	$2i$ $1f; 1h$	$1d; 1e$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; (0, 0, \frac{1}{2})$	$1a; 1b$	$2i$ $2i$	$1c; 1g$ $2i$	$1d; 1f$ $2i$	$1e; 1h$ $2\times 2i$
[2] $P\bar{1}$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; (0, 0, \frac{1}{2})$	$2i$	$1a; 1b$ $1d; 1f$	$2i$ $1c; 1g$	$2i$ $1e; 1h$	$2i$ $2\times 2i$
[p] $P\bar{1}$	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, r\mathbf{a}+\mathbf{c}$ $p = \text{prime} > 2; u = 1, \ldots p-1;$	$\frac{1}{p}(x-qy-rz), y, z; +(\frac{u}{p}, 0, 0)$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$ $-\frac{1}{2}(p-1) \le r \le \frac{1}{2}(p-1)$	$1a; \frac{p-1}{2}\times 2i$	$1b(f^{\dagger}); \frac{p-1}{2}\times 2i$ $1f(b^{\dagger}); \frac{p-1}{2}\times 2i$	$1c(e^{*}); \frac{p-1}{2}\times 2i$ $1g(h^{\ddagger}); \frac{p-1}{2}\times 2i$	$1d; \frac{p-1}{2}\times 2i$ $1h(g^{\ddagger}); \frac{p-1}{2}\times 2i$	$1e(c^{*}); \frac{p-1}{2}\times 2i$ $p\times 2i$
[p] $P\bar{1}$	$\mathbf{a}, p\mathbf{b}, q\mathbf{b}+\mathbf{c}$ $p = \text{prime} > 2; u = 1, \ldots p-1;$	$x, \frac{1}{p}(y-qz), z; +(0, \frac{u}{p}, 0)$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	$1a; \frac{p-1}{2}\times 2i$	$1b(g^{*}); \frac{p-1}{2}\times 2i$ $1f(h^{*}); \frac{p-1}{2}\times 2i$	$1c; \frac{p-1}{2}\times 2i$ $1g(b^{*}); \frac{p-1}{2}\times 2i$	$1d; \frac{p-1}{2}\times 2i$ $1h(f^{*}); \frac{p-1}{2}\times 2i$	$1e; \frac{p-1}{2}\times 2i$ $p\times 2i$
[p] $P\bar{1}$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2; u = 1, \ldots p-1$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$1a; \frac{p-1}{2}\times 2i$	$1b; \frac{p-1}{2}\times 2i$ $1f; \frac{p-1}{2}\times 2i$	$1c; \frac{p-1}{2}\times 2i$ $1g; \frac{p-1}{2}\times 2i$	$1d; \frac{p-1}{2}\times 2i$ $1h; \frac{p-1}{2}\times 2i$	$1e; \frac{p-1}{2}\times 2i$ $p\times 2i$

$^{*}\, q = 2n+1$ $\quad ^{\dagger}\, r = 2n+1$ $\quad ^{\ddagger}\, q+r = 2n+1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 3, pp. 438–439.

$P2$ No. 3 $P121$ C_2^1

UNIQUE AXIS b

	Axes	Coordinates	$1a$	$1b$	$1c$	$1d$	$2e$
I Maximal *translationengleiche* subgroups							
[2] $P1$ (1)			$1a$	$1a$	$1a$	$1a$	$2{\times}1a$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, non-isomorphic							
[2] $C121$ (5)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$	$2{\times}2a$	$2{\times}2b$	$4c$	$4c$	$2{\times}4c$
[2] $C121$ (5)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x{+}\frac{1}{4}, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$	$4c$	$4c$	$2{\times}2a$	$2{\times}2b$	$2{\times}4c$
[2] $A121$ (5)	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z;\ +(0, \frac{1}{2}, 0)$	$2{\times}2a$	$4c$	$2{\times}2b$	$4c$	$2{\times}4c$
[2] $A121$ (5)	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z{+}\frac{1}{4};{+}(0, \frac{1}{2}, 0)$	$4c$	$2{\times}2a$	$4c$	$2{\times}2b$	$2{\times}4c$
[2] $I121$ (5)	$\mathbf{a}{-}\mathbf{c}, 2\mathbf{b}, \mathbf{a}{+}\mathbf{c}$	$\frac{1}{2}(x{-}z), \frac{1}{2}y, \frac{1}{2}(x{+}z);\ +(0, \frac{1}{2}, 0)$	$2{\times}2a$	$4c$	$4c$	$2{\times}2b$	$2{\times}4c$
or: $C121$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}{+}\mathbf{c}$	$\frac{1}{2}(x{+}z), \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0);$					
[2] $I121$ (5)	$\mathbf{a}{-}\mathbf{c}, 2\mathbf{b}, \mathbf{a}{+}\mathbf{c}$	$\frac{1}{2}(x{-}z){+}\frac{1}{4}, \frac{1}{2}y, \frac{1}{2}(x{+}z){+}\frac{1}{4};\ +(0, \frac{1}{2}, 0)$	$4c$	$2{\times}2b$	$2{\times}2a$	$4c$	$2{\times}4c$
or: $C121$	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}{+}\mathbf{c}$	$\frac{1}{2}(x{+}z){+}\frac{1}{4}, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0);$					
[2] $P12_11$ (4)	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$	$2a$	$2a$	$2a$	$2a$	$2{\times}2a$
Enlarged unit cell, isomorphic							
[2] $P121$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$	$2{\times}1a$	$2{\times}1b$	$2{\times}1c$	$2{\times}1d$	$2{\times}2e$
[3] $P121$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	$3{\times}1a$	$3{\times}1b$	$3{\times}1c$	$3{\times}1d$	$3{\times}2e$
[p] $P121$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$	$p{\times}1a$	$p{\times}1b$	$p{\times}1c$	$p{\times}1d$	$p{\times}2e$
	$p = \text{prime};\ u = 1, \ldots, p-1$						
[2] $P121$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$1a; 1c$	$1b; 1d$	$2e$	$2e$	$2{\times}2e$
[2] $P121$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x{+}\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$2e$	$2e$	$1a; 1c$	$1b; 1d$	$2{\times}2e$
[2] $P121$	$\mathbf{a}{-}\mathbf{c}, \mathbf{b}, \mathbf{a}{+}\mathbf{c}$	$\frac{1}{2}(x{-}z), y, \frac{1}{2}(x{+}z);\ +(\frac{1}{2}, 0, \frac{1}{2})$	$1a; 1d$	$2e$	$2e$	$1b; 1c$	$2{\times}2e$
[2] $P121$	$\mathbf{a}{-}\mathbf{c}, \mathbf{b}, \mathbf{a}{+}\mathbf{c}$	$\frac{1}{2}(x{-}z){+}\frac{1}{4}, y, \frac{1}{2}(x{+}z){+}\frac{1}{4};\ +(\frac{1}{2}, 0, \frac{1}{2})$	$2e$	$1b; 1c$	$1a; 1d$	$2e$	$2{\times}2e$
[2] $P121$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0, 0, \frac{1}{2})$	$1a; 1b$	$2e$	$1c; 1d$	$2e$	$2{\times}2e$
[2] $P121$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z{+}\frac{1}{4};\ +(0, 0, \frac{1}{2})$	$2e$	$1a; 1b$	$2e$	$1c; 1d$	$2{\times}2e$
[3] $P121$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	$1a; 2e$	$1b; 2e$	$1c; 2e$	$1d; 2e$	$3{\times}2e$
[3] $P121$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}{+}\mathbf{c}$	$\frac{1}{3}(x{+}z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$1a; 2e$	$1d; 2e$	$1c; 2e$	$1b; 2e$	$3{\times}2e$
	or: $2\mathbf{a}{+}\mathbf{c}, \mathbf{b}, -\mathbf{a}{+}\mathbf{c}$	$\frac{1}{3}(x{+}z), y, \frac{1}{3}(-x{+}2z);\ \pm(\frac{1}{3}, 0, \frac{2}{3})$	$1a; 2e$	$1c; 2e$	$1d; 2e$	$1b; 2e$	$3{\times}2e$
[3] $P121$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}{+}\mathbf{c}$	$\frac{1}{3}(x{-}z), y, z;\ \pm(\frac{1}{3}, 0, 0)$	$1a; 2e$	$1d; 2e$	$1c; 2e$	$1b; 2e$	$3{\times}2e$
	or: $2\mathbf{a}{-}\mathbf{c}, \mathbf{b}, \mathbf{a}{+}\mathbf{c}$	$\frac{1}{3}(x{-}z), y, \frac{1}{3}(x{+}2z);\ \pm(\frac{1}{3}, 0, \frac{1}{3})$	$1a; 2e$	$1c; 2e$	$1d; 2e$	$1b; 2e$	$3{\times}2e$
[3] $P121$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	$1a; 2e$	$1b; 2e$	$1c; 2e$	$1d; 2e$	$3{\times}2e$
[p] $P121$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0, 0, \frac{u}{p})$	$1a; \frac{p-1}{2}{\times}2e$	$1b; \frac{p-1}{2}{\times}2e$	$1c; \frac{p-1}{2}{\times}2e$	$1d; \frac{p-1}{2}{\times}2e$	$p{\times}2e$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$						
[p] $P121$	$p\mathbf{a}, \mathbf{b}, q\mathbf{a}{+}\mathbf{c}$	$\frac{1}{p}(x{-}qz), y, z;\ +(\frac{u}{p}, 0, 0)$	$1a; \frac{p-1}{2}{\times}2e$	$1b(d^*);$ $\frac{p-1}{2}{\times}2e$	$1c; \frac{p-1}{2}{\times}2e$	$1d(b^*);$ $\frac{p-1}{2}{\times}2e$	$p{\times}2e$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$						

$^*\ q = 2n{+}1$

	Axes	Coordinates

I Maximal *translationengleiche* subgroups

[2] $P1$

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

[2] $A112$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $A112$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $B112$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $B112$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $I112$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$,	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$
or: $A112$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $I112$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}(-x+y)+\frac{1}{4}, \frac{1}{2}z; +(0,0,\frac{1}{2})$
or: $A112$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $P112_1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$

Enlarged unit cell, isomorphic

[2] $P112$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[3] $P112$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$
[p] $P112$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1;$	
[2] $P112$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$
[2] $P112$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$
[2] $P112$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z; +(\frac{1}{2},\frac{1}{2},0)$
[2] $P112$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}(-x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$
[2] $P112$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2},0,0)$
[2] $P112$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2},0,0)$
[3] $P112$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$
[3] $P112$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z;\ \pm(0,\frac{1}{3},0)$
	or: $\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), z;\ \pm(\frac{1}{3},\frac{2}{3},0)$
[3] $P112$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z;\ \pm(0,\frac{1}{3},0)$
	or: $\mathbf{a}+\mathbf{b}, -\mathbf{a}+2\mathbf{c}, \mathbf{c}$	$\frac{1}{3}(2x+y), \frac{1}{3}(-x+y), z;\ \pm(\frac{1}{3},\frac{1}{3},0)$
[3] $P112$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$
[p] $P112$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p},0,0)$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$	
[p] $P112$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-qx+y), z;\ +(0,\frac{u}{p},0)$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

$P2_1$ $P12_11$ No. 4 $P112_1$ C_2^2

UNIQUE AXIS b UNIQUE AXIS c

	Axes	Coordinates	Wyckoff positions $2a$		Axes	Coordinates
I Maximal *translationengleiche* subgroups						
[2] $P1$ (1)			$2\times 1a$	$P1$		
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**						
[3] $P12_11$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$3\times 2a$	$P112_1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$
[p] $P12_11$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$p\times 2a$	$P112_1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$
[2] $P12_11$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times 2a$	$P112_1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$
[2] $P12_11$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times 2a$	$P112_1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0, \frac{1}{2}, 0)$
[2] $P12_11$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$ or: $\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-z), y, \frac{1}{2}(x+z)$; $+(\frac{1}{2}, 0, \frac{1}{2})$ $x, y, \frac{1}{2}(x+z)$; $+(0, 0, \frac{1}{2})$	$2\times 2a$	$P112_1$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$ or: $2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z$; $+(\frac{1}{2}, \frac{1}{2}, 0)$ $\frac{1}{2}(x+y), y, z$; $+(\frac{1}{2}, 0, 0)$
[2] $P12_11$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$ or: $\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-z)+\frac{1}{4}, y, \frac{1}{2}(x+z)+\frac{1}{4}$; $+(\frac{1}{2}, 0, \frac{1}{2})$ $x, y, \frac{1}{2}(x+z)+\frac{1}{4}$; $+(0, 0, \frac{1}{2})$	$2\times 2a$	$P112_1$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$ or: $2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}(-x+y)+\frac{1}{4}, z$; $+(\frac{1}{2}, \frac{1}{2}, 0)$ $\frac{1}{2}(x+y)+\frac{1}{4}, y, z$; $+(\frac{1}{2}, 0, 0)$
[2] $P12_11$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0, 0, \frac{1}{2})$	$2\times 2a$	$P112_1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$
[2] $P12_11$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0, 0, \frac{1}{2})$	$2\times 2a$	$P112_1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z$; $+(\frac{1}{2}, 0, 0)$
[3] $P12_11$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times 2a$	$P112_1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$
[3] $P12_11$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times 2a$	$P112_1$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z$; $\pm(0, \frac{1}{3}, 0)$
[3] $P12_11$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times 2a$	$P112_1$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z$; $\pm(0, \frac{1}{3}, 0)$
[3] $P12_11$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$3\times 2a$	$P112_1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$
[p] $P12_11$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$p\times 2a$	$P112_1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$ p = prime; $u = 1, \ldots, p-1$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$
[p] $P12_11$	$p\mathbf{a}, \mathbf{b}, q\mathbf{a}+\mathbf{c}$ p = prime; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	$\frac{1}{p}(x-qz), y, z$; $+(\frac{u}{p}, 0, 0)$	$p\times 2a$	$P112_1$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c}$ p = prime; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	$x, \frac{1}{p}(-qx+y), z$; $+(0, \frac{u}{p}, 0)$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 5, pp. 441–443.

C_2^3 $C121$ No. 5 $A121$ $C2$

UNIQUE AXIS b

CELL CHOICE 1 | CELL CHOICE 2

	Axes	Coordinates	$2a$	$2b$	$4c$			Axes	Coordinates
I Maximal *translationengleiche* subgroups									
[2] $P1$ (1)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$	$2x, x+y, z$	$1a$	$1a$	$2\times1a$		$P1$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x, x+y, 2z$
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $P12_11$ (4)		$x+\frac{1}{4}, y, z$	$2a$	$2a$	$2\times2a$		$P12_11$		$x, y, z+\frac{1}{4}$
[2] $P121$ (3)			$1a; 1c$	$1b; 1d$	$2\times2e$				
			$1a; 1b$	$1c; 1d$	$2\times2e$	$\Rightarrow$	$P121$		
Enlarged unit cell, isomorphic									
[3] $C121$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times2b$	$3\times4c$		$A121$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$
[p] $C121$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$p\times2a$	$p\times2b$	$p\times4c$		$A121$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$
	p = prime > 2; $u = 1, \ldots, p-1$							p = prime > 2; $u = 1, \ldots, p-1$	
[2] $C121$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$2a; 2b$	$4c$	$2\times4c$		$A121$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$
[2] $C121$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$	$4c$	$2a; 2b$	$2\times4c$		$A121$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[2] $I121$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$2a; 2b$	$4c$	$2\times4c$		$I121$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$
[2] $I121$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$	$4c$	$2a; 2b$	$2\times4c$		$I121$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[3] $C121$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$2a; 4c$	$2b; 4c$	$3\times4c$		$A121$	$\mathbf{a}+\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(-x+z); \pm(0, 0, \frac{1}{3})$
[3] $C121$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z; \pm(\frac{1}{3}, 0, 0)$	$2a; 4c$	$2b; 4c$	$3\times4c$		$A121$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(x+z); \pm(0, 0, \frac{1}{3})$
[3] $C121$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z; \pm(\frac{1}{3}, 0, 0)$	$2a; 4c$	$2b; 4c$	$3\times4c$		$A121$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$
[3] $C121$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$2a; 4c$	$2b; 4c$	$3\times4c$		$A121$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$
[p] $C121$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$2a; \frac{p-1}{2}\times 4c$	$2b; \frac{p-1}{2}\times 4c$	$p\times4c$		$A121$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$
	p = prime > 2; $u = 1, \ldots, p-1$							p = prime > 2; $u = 1, \ldots, p-1$	
[p] $C121$	$p\mathbf{a}, \mathbf{b}, q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z; +(\frac{u}{p}, 0, 0)$	$2a; \frac{p-1}{2}\times 4c$	$2b; \frac{p-1}{2}\times 4c$	$p\times4c$		$A121$	$\mathbf{a}+q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}(-qx+z); +(0, 0, \frac{u}{p})$
	p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$							p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	

For cell choice 3 see next page

	Axes	Coordinates	Wyckoff positions 2a	2b	4c		Axes	Coordinates
I Maximal *translationengleiche* subgroups								
[2] $P1$ (1)	$\mathbf{a}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c}), \mathbf{c}$	$x+y, 2y, y+z$	$1a$	$1a$	$2\times1a$	$P1$ (1)	$\mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c}), \mathbf{c}$	$x, 2y, y+z$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P12_11$ (4)		$x-\frac{1}{4}, y, z-\frac{1}{4}$	$2a$	$2a$	$2\times2a$	$P112_1$ (4)		$x, y+\frac{1}{4}, z$
[2] $P121$ (3)			$1a; 1d$	$1b; 1c$	$2\times2e$			
			$1a; 1c$	$1b; 1d$	$2\times2e$	$\Rightarrow$ $P112$ (3)		
			$1a; 1b$	$1c; 1d$	$2\times2e$	$\Longrightarrow$		
Enlarged unit cell, isomorphic								
[3] $I121$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times2b$	$3\times4c$	$A112$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$
[p] $I121$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$p\times2a$	$p\times2b$	$p\times4c$	$A112$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$						$p = \text{prime} > 2;\ u = 1, \ldots, p-1$	
[2] $I121$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), y, z; +(\frac{1}{2}, 0, 0)$	$2a; 2b$	$4c$	$2\times4c$	$A112$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$
[2] $I121$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z)+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	$4c$	$2a; 2b$	$2\times4c$	$A112$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[2] $I121$	$2\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, z; +(\frac{1}{2}, 0, 0)$	$2a; 2b$	$4c$	$2\times4c$	$I112$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$
[2] $I121$	$2\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z)+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	$4c$	$2a; 2b$	$2\times4c$	$I112$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[3] $I121$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$2a; 4c$	$2b; 4c$	$3\times4c$	$A112$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$
[3] $A121$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z; \pm(\frac{1}{3}, 0, 0)$	$2a; 4c$	$2b; 4c$	$3\times4c$	$A112$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z; \pm(0, \frac{1}{3}, 0)$
[3] $I121$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$2a; 4c$	$2b; 4c$	$3\times4c$	$A112$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z; \pm(0, \frac{1}{3}, 0)$
[3] $A121$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z; \pm(\frac{1}{3}, 0, 0)$	$2a; 4c$	$2b; 4c$	$3\times4c$	$A112$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$
[p] $I121$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; \pm(\frac{u}{p}, 0, 0)$	$2a; \frac{p-1}{2}\times 4c$	$2b; \frac{p-1}{2}\times 4c$	$p\times4c$	$A112$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$						$p = \text{prime} > 2;\ u = 1, \ldots, p-1$	
[p] $I121$	$\mathbf{a}+2q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}(-2qx+z); +(0, 0, \frac{u}{p})$	$2a; \frac{p-1}{2}\times 4c$	$2b; \frac{p-1}{2}\times 4c$	$p\times4c$	$A112$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-qx+y), z; +(0, \frac{u}{p}, 0)$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$						$p = \text{prime} > 2;\ u = 1, \ldots, p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

For unique axis **b**, *cell choices* 1 *and* 2, *see preceding page*

	Axes	Coordinates		Axes	Coordinates

I Maximal *translationengleiche* subgroups

[2] $P1$	$\frac{1}{2}(\mathbf{a}-\mathbf{c}), \mathbf{b}, \mathbf{c}$	$2x, y, y+z$	$P1$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$x+z, y+z, 2z$

II Maximal *klassengleiche* subgroups

Loss of centring translations

[2] $P112_1$		$x+\frac{1}{4}, y, z$	$P112_1$		$x-\frac{1}{4}, y-\frac{1}{4}, z$
[2]			$P112$		
[2] $P112$					

Enlarged unit cell, isomorphic

[3] $B112$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}, z;\ \pm(0,0,\frac{1}{3})$	$I112$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$
[p] $B112$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2;\ u = 1,\dots,p-1$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$I112$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2;\ u = 1,\dots,p-1$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$
[2] $B112$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0,\frac{1}{2},0)$	$I112$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z;\ +(0,\frac{1}{2},0)$
[2] $B112$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y-\frac{1}{4}, z;\ +(0,\frac{1}{2},0)$	$I112$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y)+\frac{1}{4}, z;\ +(0,\frac{1}{2},0)$
[2] $I112$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0,\frac{1}{2},0)$	$I112$	$\mathbf{a}+\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(-x+y), z;\ +(0,\frac{1}{2},0)$
[2] $I112$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y-\frac{1}{4}, z;\ +(0,\frac{1}{2},0)$	$I112$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y-\frac{1}{4}, z;\ +(0,\frac{1}{2},0)$
[3] $B112$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x-y), y, z;\ \pm(\frac{1}{3},0,0)$	$I112$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3},0,0)$
[3] $B112$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), y, z;\ \pm(\frac{1}{3},0,0)$	$B112$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z;\ \pm(0,\frac{1}{3},0)$
[3] $B112$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3},0,0)$	$I112$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0,\frac{1}{3},0)$
[3] $B112$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0,\frac{1}{3},0)$	$B112$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z;\ \pm(0,\frac{1}{3},0)$
[p] $B112$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 2;\ u = 1,\dots,p-1$	$x, \frac{1}{p}y, z;\ +(0,\frac{u}{p},0)$	$I112$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 2;\ u = 1,\dots,p-1$	$x, \frac{1}{p}y, z;\ \pm(0,\frac{u}{p},0)$
[p] $B112$	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 2;\ u = 1,\dots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	$\frac{1}{p}(x-qy), y, z;\ +(0,\frac{u}{p},0)$	$I112$	$p\mathbf{a}, 2q\mathbf{a}+\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 2;\ u = 1,\dots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	$\frac{1}{p}(x-2qy), y, z;\ +(\frac{u}{p},0,0)$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 6, pp. 444–445.

Pm No. 6 $P1m1$ C_s^1

UNIQUE AXIS b

	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$2c$
I Maximal *translationengleiche* subgroups					
[2] $P1$ (1)			$1a$	$1a$	$2\times1a$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[2] $C1m1$ (8)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$2\times2a$	$4b$	$2\times4b$
[2] $C1m1$ (8)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$	$4b$	$2\times2a$	$2\times4b$
[2] $C1m1$ (8)	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$2\times2a$	$4b$	$2\times4b$
[2] $C1m1$ (8)	$2\mathbf{a}, 2\mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), \frac{1}{2}y+\frac{1}{4}, z;$	$4b$	$2\times2a$	$2\times4b$
[2] $A1m1$ (8)	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,\frac{1}{2},0);$	$2\times2a$	$4b$	$2\times4b$
[2] $A1m1$ (8)	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,\frac{1}{2},0)$	$4b$	$2\times2a$	$2\times4b$
[2] $P1a1$ (7)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2},0,0)$	$2a$	$2a$	$2\times2a$
[2] $P1c1$ (7)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2a$	$2\times2a$
[2] $P1c1$ (7)	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z); +(0,0,\frac{1}{2})$	$2a$	$2a$	$2\times2a$
Enlarged unit cell, isomorphic					
[2] $P1m1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$1a; 1b$	$2c$	$2\times2c$
[2] $P1m1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$	$2c$	$1a; 1b$	$2\times2c$
[3] $P1m1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$	$1a; 2c$	$1b; 2c$	$3\times2c$
[p] $P1m1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0,\frac{u}{p},0)$	$1a; \frac{p-1}{2}\times2c$	$1b; \frac{p-1}{2}\times2c$	$p\times2c$
	p = prime > 2; $u = 1,\ldots,p-1$				
[2] $P1m1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2},0,0)$	$2\times1a$	$2\times1b$	$2\times2c$
[2] $P1m1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, \frac{1}{2}(x+z); +(\frac{1}{2},0,\frac{1}{2})$	$2\times1a$	$2\times1b$	$2\times2c$
[2] $P1m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2\times1a$	$2\times1b$	$2\times2c$
[3] $P1m1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$	$3\times1a$	$3\times1b$	$3\times2c$
[3] $P1m1$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z; \pm(\frac{1}{3},0,0)$	$3\times1a$	$3\times1b$	$3\times2c$
[3] $P1m1$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z; \pm(\frac{1}{3},0,0)$	$3\times1a$	$3\times1b$	$3\times2c$
[3] $P1m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times1a$	$3\times1b$	$3\times2c$
[p] $P1m1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times1a$	$p\times1b$	$p\times2c$
	p = prime > 2; $u = 1,\ldots,p-1$				
[p] $P1m1$	$p\mathbf{a}, \mathbf{b}, q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z; +(\frac{u}{p},0,0)$	$p\times1a$	$p\times1b$	$p\times2c$
	p = prime > 2; $u = 1,\ldots,p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$				

	Axes	Coordinates

I Maximal *translationengleiche* subgroups

[2] $P1$

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

[2] $A11m$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $A11m$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
[2] $A11m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $A11m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
[2] $B11m$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $B11m$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
[2] $P11b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$
[2] $P11a$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2},0,0)$
[2] $P11a$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), y, z; +(\frac{1}{2},0,0)$

Enlarged unit cell, isomorphic

[2] $P11m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $P11m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
[3] $P11m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$
[p] $P11m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$	
[2] $P11m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$
[2] $P11m$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z; +(\frac{1}{2},\frac{1}{2},0)$
[2] $P11m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2},0,0)$
[3] $P11m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$
[3] $P11m$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z; \pm(0,\frac{1}{3},0)$
[3] $P11m$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z; \pm(0,\frac{1}{3},0)$
[3] $P11m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$
[p] $P11m$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p},0,0)$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$	
[p] $P11m$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-qx+y), z; +(0,\frac{u}{p},0)$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 7, pp. 446–447.

Pc $P1c1$ No. 7 $P1n1$ $P1a1$ C_s^2

UNIQUE AXIS b

CELL CHOICE 1				CELL CHOICE 2			CELL CHOICE 3		
	Axes	Coordinates	Wyckoff positions 2a		Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups									
[2] $P1$ (1)			$2\times 1a$	$P1$			$P1$		
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $C1c1$ (9)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$2\times 4a$	$A1n1$	$\mathbf{a}-\mathbf{c}$, $2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}(x+z)$; $+(0, \frac{1}{2}, 0)$	$I1a1$	$\mathbf{a}, 2\mathbf{b}$, $\mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z, \frac{1}{2}y, \frac{1}{2}z$; $+(0, \frac{1}{2}, 0)$
[2] $C1c1$ (9)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0, \frac{1}{2}, 0)$	$2\times 4a$	$A1n1$	$\mathbf{a}-\mathbf{c}$, $2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}(x+z)$; $+(0, \frac{1}{2}, 0)$	$I1a1$	$\mathbf{a}, 2\mathbf{b}$, $\mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z$; $+(0, \frac{1}{2}, 0)$
Enlarged unit cell, isomorphic									
[2] $P1c1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$2\times 2a$	$P1n1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$P1a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$
[2] $P1c1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0, \frac{1}{2}, 0)$	$2\times 2a$	$P1n1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0, \frac{1}{2}, 0)$	$P1a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0, \frac{1}{2}, 0)$
[3] $P1c1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$3\times 2a$	$P1n1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$P1a1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$
[p] $P1c1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$; p = prime; $u = 1, \ldots, p-1$	$p\times 2a$	$P1n1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$; p = prime; $u = 1, \ldots, p-1$	$P1a1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$; p = prime; $u = 1, \ldots, p-1$
[2] $P1c1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times 2a$	$P1n1$	$\mathbf{a}-\mathbf{c}$, $\mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z)$; $+(0, 0, \frac{1}{2})$	$P1a1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0, 0, \frac{1}{2})$
[2] $P1n1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times 2a$	$P1a1$	$\mathbf{a}-\mathbf{c}$, $\mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z)$; $+(0, 0, \frac{1}{2})$	$P1n1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0, 0, \frac{1}{2})$
[3] $P1c1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times 2a$	$P1n1$	$\mathbf{a}-2\mathbf{c}$, $\mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(2x+z)$; $\pm(0, 0, \frac{1}{3})$	$P1a1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$
[3] $P1c1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$3\times 2a$	$P1n1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$P1a1$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $P1c1$	$\mathbf{a}+\mathbf{c}$, $\mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(-x+z)$; $\pm(0, 0, \frac{1}{3})$	$3\times 2a$	$P1n1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$P1a1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $P1c1$	$\mathbf{a}-\mathbf{c}$, $\mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(x+z)$; $\pm(0, 0, \frac{1}{3})$	$3\times 2a$	$P1n1$	$2\mathbf{a}+\mathbf{c}, \mathbf{b}$, $\mathbf{a}+2\mathbf{c}$	$\frac{1}{3}(2x-z), y, \frac{1}{3}(-x+2z)$; $\pm(\frac{1}{3}, 0, \frac{1}{3})$	$P1a1$	$3\mathbf{a}, \mathbf{b}$, $-\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z$; $\pm(\frac{1}{3}, 0, 0)$
[p] $P1c1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$; p = prime; $u = 1, \ldots, p-1$;	$p\times 2a$	$P1n1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$; p = prime; $u = 1, \ldots, p-1$;	$P1a1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$; p = prime; $u = 1, \ldots, p-1$;
[p] $P1c1$	$\mathbf{a}+q\mathbf{c}$, $\mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}(-qx+z)$; $+(0, 0, \frac{u}{p})$; p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$p\times 2a$	$P1n1$	$p\mathbf{a}, \mathbf{b}$, $2q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-2qz), y, z$; $+(\frac{u}{p}, 0, 0)$; p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$P1a1$	$p\mathbf{a}, \mathbf{b}$, $q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z$; $+(\frac{u}{p}, 0, 0)$; p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

$P11a$ No. 7 $P11n$ $P11b$ Pc

UNIQUE AXIS c

CELL CHOICE 1 — CELL CHOICE 2 — CELL CHOICE 3

	Axes	Coordinates	Wyckoff positions $2a$		Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups									
[2] $P1$ (1)			$2\times 1a$	$P1$			$P1$		
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $A11a$ (9)	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$x,\frac{1}{2}y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2\times 4a$	$B11n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x+y),y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$I11b$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x,-\frac{1}{2}x+y,\frac{1}{2}z;+(0,0,\frac{1}{2})$
[2] $A11a$ (9)	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$x,\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$2\times 4a$	$B11n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x+y),y,\frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$I11b$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x,-\frac{1}{2}x+y,\frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
Enlarged unit cell, isomorphic									
[2] $P11a$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2\times 2a$	$P11n$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$P11b$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$
[2] $P11a$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$2\times 2a$	$P11n$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$P11b$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$
[3] $P11a$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$3\times 2a$	$P11n$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$P11b$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$
[p] $P11a$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$; $p=$ prime; $u=1,\dots,p-1$	$p\times 2a$	$P11n$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$; $p=$ prime; $u=1,\dots,p-1$	$P11b$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$; $p=$ prime; $u=1,\dots,p-1$
[2] $P11a$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;+(0,\frac{1}{2},0)$	$2\times 2a$	$P11n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x+y),y,z;+(\frac{1}{2},0,0)$	$P11b$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;+(\frac{1}{2},0,0)$
[2] $P11n$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;+(0,\frac{1}{2},0)$	$2\times 2a$	$P11b$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x+y),y,z;+(\frac{1}{2},0,0)$	$P11n$	$2a,\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;+(\frac{1}{2},0,0)$
[3] $P11a$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$3\times 2a$	$P11n$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+2y),y,z; \pm(\frac{1}{3},0,0)$	$P11b$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$
[3] $P11a$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$3\times 2a$	$P11n$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$P11b$	$\mathbf{a}+\mathbf{b},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}(-x+y),z;\pm(0,\frac{1}{3},0)$
[3] $P11a$	$3\mathbf{a}, \mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x-y),y,z; \pm(\frac{1}{3},0,0)$	$3\times 2a$	$P11n$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$P11b$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$
[3] $P11a$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+y),y,z; \pm(\frac{1}{3},0,0)$	$3\times 2a$	$P11n$	$2\mathbf{a}+\mathbf{b}, \mathbf{a}+2\mathbf{b},\mathbf{c}$	$\frac{1}{3}(2x-y),\frac{1}{3}(-x+2y),z; \pm(\frac{1}{3},\frac{1}{3},0)$	$P11b$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}(x+y),z; \pm(0,\frac{1}{3},0)$
[p] $P11a$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$; $p=$ prime; $u=1,\dots,p-1$;	$p\times 2a$	$P11n$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$; $p=$ prime; $u=1,\dots,p-1$;	$P11b$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$; $p=$ prime; $u=1,\dots,p-1$;
[p] $P11a$	$p\mathbf{a}, q\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{p}(x-qy),y,z; +(\frac{u}{p},0,0)$; $p=$ prime >2; $u=1,\dots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$	$p\times 2a$	$P11n$	$\mathbf{a}+2q\mathbf{b}, p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}(-2qx+y),z; +(0,\frac{u}{p},0)$; $p=$ prime >2; $u=1,\dots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$	$P11b$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}(-qx+y),z; +(0,\frac{u}{p},0)$; $p=$ prime >2; $u=1,\dots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 8, pp. 448–449.

Cm $C1m1$ No. 8 $A1m1$ $I1m1$ C_s^3

UNIQUE AXIS b

CELL CHOICE 1 | CELL CHOICE 2 | CELL CHOICE 3

	Axes	Coordinates	Wyckoff positions $2a$	$4b$	Cell choice 2	Axes	Coordinates	Cell choice 3	Axes	Coordinates
I Maximal *translationengleiche* subgroups										
[2] $P1$ (1)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\mathbf{b}$, $\mathbf{c}$	$2x, x+y, z$;	$1a$	$2\times1a$	$P1$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x, x+y, 2z$	$P1$	$\mathbf{a}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$, $\mathbf{c}$	$x+y, 2y, y+z$
II Maximal *klassengleiche* subgroups										
Loss of centring translations										
[2] $P1a1$ (7)		$x, y+\frac{1}{4}, z$	$2a$	$2\times2a$	$P1c1$		$x, y+\frac{1}{4}, z$	$P1n1$		$x, y+\frac{1}{4}, z$
[2] $P1m1$ (6)			$1a$; $1b$	$2\times2c$	$P1m1$			$P1m1$		
Enlarged unit cell, non-isomorphic										
[2] $C1c1$ (9)	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a$	$2\times4a$	$A1n1$	$2\mathbf{a}+\mathbf{c}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, y, -\frac{1}{2}x+z$; $+(\frac{1}{2},0,0)$	$I1a1$	$2\mathbf{a}$, $\mathbf{b}$, $-\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), y, z$; $+(\frac{1}{2},0,0)$
[2] $C1c1$ (9)	$\mathbf{a}-2\mathbf{c}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, x+\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a$	$2\times4a$	$I1a1$	$2\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2},0,0)$	$I1a1$	$2\mathbf{a}$, $\mathbf{b}$, $\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, z$; $+(\frac{1}{2},0,0)$
$\widehat{=}$ $I1a1$	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y+\frac{1}{4}, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$								
Enlarged unit cell, isomorphic										
[3] $C1m1$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$	$2a$; $4b$	$3\times4b$	$A1m1$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$	$I1m1$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$
[p] $C1m1$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$	$2a$; $\frac{p-1}{2}\times4b$	$p\times4b$	$A1m1$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$	$I1m1$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$
		$p =$ prime > 2; $u = 1,\ldots,p-1$					$p =$ prime > 2; $u = 1,\ldots,p-1$			$p =$ prime > 2; $u = 1,\ldots,p-1$
[2] $C1m1$	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2\times2a$	$2\times4b$	$A1m1$	$2\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2},0,0)$	$I1m1$	$2\mathbf{a}$, $\mathbf{b}$, $-\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), y, z$; $+(\frac{1}{2},0,0)$
[2] $I1m1$	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2\times2a$	$2\times4b$	$I1m1$	$2\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2},0,0)$	$I1m1$	$2\mathbf{a}$, $\mathbf{b}$, $\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, z$; $+(\frac{1}{2},0,0)$
[3] $C1m1$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$	$3\times2a$	$3\times4b$	$A1m1$	$\mathbf{a}+\mathbf{c}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}(-x+z)$; $\pm(0,0,\frac{1}{3})$	$I1m1$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$
[3] $C1m1$	$3\mathbf{a}$, $\mathbf{b}$, $-\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z$; $\pm(\frac{1}{3},0,0)$	$3\times2a$	$3\times4b$	$A1m1$	$\mathbf{a}-\mathbf{c}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}(x+z)$; $\pm(0,0,\frac{1}{3})$	$I1m1$	$3\mathbf{a}$, $\mathbf{b}$, $2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-2z), y, z$; $\pm(\frac{1}{3},0,0)$
[3] $C1m1$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z$; $\pm(\frac{1}{3},0,0)$	$3\times2a$	$3\times4b$	$A1m1$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$I1m1$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$
[3] $C1m1$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times4b$	$A1m1$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $+(\frac{1}{3},0,0)$	$I1m1$	$3\mathbf{a}$, $\mathbf{b}$, $-2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+2z), y, z$; $\pm(\frac{1}{3},0,0)$
[p] $C1m1$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times2a$	$p\times4b$	$A1m1$	$p\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p},0,0)$	$I1m1$	$p\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}x, y, z$; $\pm(\frac{u}{p},0,0)$
		$p =$ prime; $u = 1,\ldots,p-1$					$p =$ prime; $u = 1,\ldots,p-1$			$p =$ prime; > 2; $u = 1,\ldots,p-1$
[p] $C1m1$	$p\mathbf{a}$, $\mathbf{b}$, $q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z$; $+(\frac{u}{p},0,0)$	$p\times2a$	$p\times4b$	$A1m1$	$\mathbf{a}+q\mathbf{c}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}(-qx+z)$; $+(0,0,\frac{u}{p})$	$I1m1$	$\mathbf{a}+2q\mathbf{c}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}(-2qx+z)$; $+(0,0,\frac{u}{p})$
		$p =$ prime > 2; $u = 1,\ldots,p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$					$p =$ prime > 2; $u = 1,\ldots,p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$			$p =$ prime > 2; $u = 1,\ldots,p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$

CELL CHOICE 1 | CELL CHOICE 2 | CELL CHOICE 3

	Axes	Coordinates	Wyckoff positions $2a$	$4b$		Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups										
[2] $P1$ (1)	$\mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c}), \mathbf{c}$	$x, 2y, y+z$;	$1a$	$2\times1a$	$P1$	$\frac{1}{2}(\mathbf{a}-\mathbf{c}), \mathbf{b}, \mathbf{c}$	$2x, y, y+z$	$P1$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$x+z, y+z, 2z$
II Maximal *klassengleiche* subgroups										
Loss of centring translations										
[2] $P11b$ (7)		$x, y, z+\frac{1}{4}$	$2a$	$2\times2a$	$P11a$		$x, y, z+\frac{1}{4}$	$P11n$		$x, y, z+\frac{1}{4}$
[2] $P11m$ (6)			$1a; 1b$	$2\times2c$	$P11m$			$P11m$		
Enlarged unit cell, non-isomorphic										
[2] $A11a$ (9)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$4a$	$2\times4a$	$B11n$	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11b$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z$; $+(0, \frac{1}{2}, 0)$
[2] $A11a$ (9)	$2\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+y, y, z$; $+(\frac{1}{2}, 0, 0)$	$4a$	$2\times4a$	$I11b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11b$	$\mathbf{a}+\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(-z+y), z$; $+(0, \frac{1}{2}, 0)$
$\widehat{=}\, I11b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z+\frac{1}{4}$; $+(\frac{1}{2}, 0, 0)$								
Enlarged unit cell, isomorphic										
[3] $A11m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$2a; 4b$	$3\times4b$	$B11m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$I11m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$
[p] $A11m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$2a; \frac{p-1}{2}\times4b$	$p\times4b$	$B11m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$I11m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$
$p=$ prime >2; $u=1,\ldots,p-1$					$p=$ prime >2; $u=1,\ldots,p-1$			$p=$ prime >2; $u=1,\ldots,p-1$		
[2] $A11m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times2a$	$2\times4b$	$B11m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z$; $+(0, \frac{1}{2}, 0)$
[2] $I11m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2\times2a$	$2\times4b$	$I11m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0, \frac{1}{2}, 0)$	$I11m$	$\mathbf{a}+\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(-x+y), z$; $+(0, \frac{1}{2}, 0)$
[3] $A11m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times4b$	$B11m$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x-y), y, z$; $\pm(\frac{1}{3}, 0, 0)$	$I11m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $A11m$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z$; $\pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times4b$	$B11m$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), y, z$; $\pm(\frac{1}{3}, 0, 0)$	$I11m$	$\mathbf{a}+2\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-2x+y), z$; $\pm(0, \frac{1}{3}, 0)$
[3] $A11m$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z$; $\pm(0, \frac{1}{3}, 0)$	$3\times2a$	$3\times4b$	$B11m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$I11m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$
[3] $A11m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times2a$	$3\times4b$	$B11m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $+(0, \frac{1}{3}, 0)$	$I11m$	$\mathbf{a}-2\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(2x+y), z$; $\pm(0, \frac{1}{3}, 0)$
[p] $A11m$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$	$p\times2a$	$p\times4b$	$B11m$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$I11m$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $\pm(0, \frac{u}{p}, 0)$
$p=$ prime; $u=1,\ldots,p-1$					$p=$ prime; $u=1,\ldots,p-1$			$p=$ prime; >2; $u=1,\ldots,p-1$		
[p] $A11m$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-qx+y), z$; $+(0, \frac{u}{p}, 0)$	$p\times2a$	$p\times4b$	$B11m$	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(x-qy), y, z$; $+(\frac{u}{p}, 0, 0)$	$I11m$	$p\mathbf{a}, 2q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(x-2qy), y, z$; $+(\frac{u}{p}, 0, 0)$
$p=$ prime >2; $u=1,\ldots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$					$p=$ prime >2; $u=1,\ldots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$			$p=$ prime >2; $u=1,\ldots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$		

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 9, pp. 450–451.

Cc $C1c1$ No. 9 $A1n1$ $I1a1$ C_s^4

UNIQUE AXIS b

CELL CHOICE 1 | CELL CHOICE 2 | CELL CHOICE 3

	Axes	Coordinates	Wyckoff positions $4a$		Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups									
[2] $P1$ (1)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\mathbf{b}$, $\mathbf{c}$	$2x, x+y, z$	$2\times 2a$	$P1$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x, x+y, 2z$	$P1$	$\mathbf{a}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$, $\mathbf{c}$	$x+y, 2y, y+z$
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $P1c1$ (7)			$2\times 2a$	$P1n1$			$P1a1$		
[2] $P1n1$ (7)		$x, y+\frac{1}{4}, z$	$2\times 2a$	$P1a1$		$x, y+\frac{1}{4}, z$	$P1c1$		$x, y+\frac{1}{4}, z$
Enlarged unit cell, isomorphic									
[3] $C1c1$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$3\times 4a$	$A1n1$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$I1a1$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$
[p] $C1c1$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$p\times 4a$	$A1n1$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$I1a1$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$
[3] $C1c1$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times 4a$	$A1n1$	$\mathbf{a}-2\mathbf{c}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}(2x+z)$; $\pm(0, 0, \frac{1}{3})$	$I1a1$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$
[3] $C1c1$	$3\mathbf{a}$, $\mathbf{b}$, $2\mathbf{a}+\mathbf{c}$ or: $3\mathbf{a}$, $\mathbf{b}$, $-\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-2z), y, z$; $\pm(\frac{1}{3}, 0, 0)$ $\frac{1}{3}(x+z), y+\frac{1}{4}, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times 4a$	$A1n1$	$\mathbf{a}+2\mathbf{c}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}(-2x+z)$; $\pm(0, 0, \frac{1}{3})$	$I1a1$	$3\mathbf{a}$, $\mathbf{b}$, $2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-2z), y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $C1c1$	$3\mathbf{a}$, $\mathbf{b}$, $-2\mathbf{a}+\mathbf{c}$ or: $3\mathbf{a}$, $\mathbf{b}$, $\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+2z), y, z$; $\pm(\frac{1}{3}, 0, 0)$ $\frac{1}{3}(x-z), y+\frac{1}{4}, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times 4a$	$A1n1$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$I1a1$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $C1c1$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$3\times 4a$	$A1n1$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$I1a1$	$3\mathbf{a}$, $\mathbf{b}$, $-2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+2z), y, z$; $\pm(\frac{1}{3}, 0, 0)$
[p] $C1c1$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$p\times 4a$	$A1n1$	$p\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$	$I1a1$	$p\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$
[p] $C1c1$	$p\mathbf{a}$, $\mathbf{b}$, $2q\mathbf{a}+\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$\frac{1}{p}(x-2qz), y, z$; $+(\frac{u}{p}, 0, 0)$	$p\times 4a$	$A1n1$	$\mathbf{a}+2q\mathbf{c}$, $\mathbf{b}$, $p\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$x, y, \frac{1}{p}(-2qx+z)$; $+(0, 0, \frac{u}{p})$	$I1a1$	$\mathbf{a}+2q\mathbf{c}$, $\mathbf{b}$, $p\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$x, y, \frac{1}{p}(-2qx+z)$; $+(0, 0, \frac{u}{p})$

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

CELL CHOICE 1 | CELL CHOICE 2 | CELL CHOICE 3

	Axes	Coordinates	Wyckoff positions $2a$		Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups									
[2] $P1$	$\mathbf{a}$, $\frac{1}{2}(\mathbf{b}-\mathbf{c})$, $\mathbf{c}$	$x, 2y, y+z$	$2\times 2a$	$P1$	$\frac{1}{2}(\mathbf{a}-\mathbf{c})$, $\mathbf{b}$, $\mathbf{c}$	$2x, y, y+z$	$P1$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$x+y, y+z, 2z$
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $P11a$			$2\times 2a$	$P11n$			$P11b$		
[2] $P11n$		$x, y, z+\frac{1}{4}$	$2\times 2a$	$P11b$		$x, y, z+\frac{1}{4}$	$P11a$		$x, y, z+\frac{1}{4}$
Enlarged unit cell, isomorphic									
[3] $A11a$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times 4a$	$B11n$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$I11b$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$
[p] $A11a$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime > 2; $u = 1,\dots,p-1$	$p\times 4a$	$B11n$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime > 2; $u = 1,\dots,p-1$	$I11b$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime > 2; $u = 1,\dots,p-1$
[3] $A11a$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$	$3\times 4a$	$B11n$	$3\mathbf{a}$, $-2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}(x+2y), y, z$; $\pm(\frac{1}{3},0,0)$	$I11b$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$
[3] $A11a$	$\mathbf{a}+2\mathbf{b}$, $3\mathbf{b}$, $\mathbf{c}$ or: $\mathbf{a}-\mathbf{b}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}(-2x+y), z$; $\pm(0,\frac{1}{3},0)$ $x, \frac{1}{3}(x+y), z+\frac{1}{4}$; $\pm(0,\frac{1}{3},0)$	$3\times 4a$	$B11n$	$3\mathbf{a}$, $2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}(x-2y), y, z$; $\pm(\frac{1}{3},0,0)$	$I11b$	$\mathbf{a}+2\mathbf{b}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}(-2x+y), z$; $\pm(0,\frac{1}{3},0)$
[3] $A11a$	$\mathbf{a}-2\mathbf{b}$, $3\mathbf{b}$, $\mathbf{c}$ or: $\mathbf{a}+\mathbf{b}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}(2x+y), z$; $\pm(0,\frac{1}{3},0)$ $x, \frac{1}{3}(-z+y), z+\frac{1}{4}$; $\pm(0,\frac{1}{3},0)$	$3\times 4a$	$B11n$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$	$I11b$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$
[3] $A11a$	$3\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$	$3\times 4a$	$B11n$	$\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$	$I11b$	$\mathbf{a}-2\mathbf{b}$, $3\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{3}(2x+y), z$; $\pm(0,\frac{1}{3},0)$
[p] $A11a$	$p\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p},0,0)$ p = prime > 2; $u = 1,\dots,p-1$	$p\times 4a$	$B11n$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$ p = prime > 2; $u = 1,\dots,p-1$	$I11b$	$\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$ p = prime > 2; $u = 1,\dots,p-1$
[p] $A11a$	$\mathbf{a}+2q\mathbf{b}$, $p\mathbf{b}$, $\mathbf{c}$	$x, \frac{1}{p}(-2qx+y), z$; $+(0,\frac{u}{p},0)$ p = prime > 2; $u = 1,\dots,p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	$p\times 4a$	$B11n$	$p\mathbf{a}$, $2q\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}(x-2qy), y, z$; $+(\frac{u}{p},0,0)$ p = prime > 2; $u = 1,\dots,p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	$I11b$	$p\mathbf{a}$, $2q\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}(x-2qy), y, z$; $+(\frac{u}{p},0,0)$ p = prime > 2; $u = 1,\dots,p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

$P2/m$ No. 10 $P12/m1$ C_{2h}^1

UNIQUE AXIS b

Subgroup	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$1c$	$1d$	$1e$	$1f$ $2k$	$1g$ $2l$	$1h$ $2m$	$2i$ $2n$	$2j$ $4o$
I Maximal *translationengleiche* subgroups												
[2] $P1m1$ (6)			$1a$	$1b$	$1a$	$1a$	$1b$	$1b$ $2c$	$1a$ $2c$	$1b$ $2\times1a$	$2c$ $2\times1b$	$2c$ $2\times2c$
[2] $P121$ (3)			$1a$	$1a$	$1b$	$1c$	$1c$	$1b$ $2\times1b$	$1d$ $2\times1d$	$1d$ $2e$	$2\times1a$ $2e$	$2\times1c$ $2\times2e$
[2] $P\bar{1}$ (2)			$1a$	$1c(b^*)$	$1b(d^*)$	$1d(c^*)$	$1e(g^*)$	$1g(f^*)$ $2i$	$1f(e^*)$ $2i$	$1h$ $2i$	$2i$ $2i$	$2i$ $2\times2i$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**												
[2] $P12/a1$ (13)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z$; $+(\frac{1}{2},0,0)$	$2a$	$2c$	$2d$	$2e$	$2e$	$2b$ $4g$	$2f$ $2\times2f$	$2f$ $4g$	$4g$ $4g$	$2\times2e$ $2\times4g$
[2] $P12/a1$ (13)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z$; $+(\frac{1}{2},0,0)$	$2e$	$2e$	$2f$	$2a$	$2c$	$2f$ $2\times2f$	$2d$ $4g$	$2b$ $4g$	$2\times2e$ $4g$	$4g$ $2\times4g$
[2] $P12/c1$ (13)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a$	$2c$	$2e$	$2d$	$2b$	$2e$ $2\times2e$	$2f$ $2\times2f$	$2f$ $4g$	$4g$ $4g$	$4g$ $2\times4g$
[2] $P12/c1$ (13)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2e$	$2e$	$2a$	$2f$	$2f$	$2c$ $4g$	$2d$ $4g$	$2b$ $4g$	$2\times2e$ $4g$	$2\times2f$ $2\times4g$
[2] $P12/c1$ (13)	**a**–**c**, **b**, 2**c**	$x,y,\frac{1}{2}(x+z)$; $+(0,0,\frac{1}{2})$	$2a$	$2c$	$2e$	$2f$	$2f$	$2e$ $2\times2e$	$2d$ $4g$	$2b$ $4g$	$4g$ $4g$	$2\times2f$ $2\times4g$
or: $P12/n1$	**a**–**c**, **b**, **a**+**c**	$\frac{1}{2}(x-z),y,\frac{1}{2}(x+z)$; $+(\frac{1}{2},0,\frac{1}{2})$	$2a$	$2c$	$2f$	$2e$	$2e$	$2f$ $2\times2f$	$2d$ $4g$	$2b$ $4g$	$4g$ $4g$	$2\times2e$ $2\times4g$
[2] $P12/c1$ (13)	**a**–**c**, **b**, 2**c**	$x,y,\frac{1}{2}(x+z)+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2e$	$2e$	$2a$	$2d$	$2b$	$2c$ $4g$	$2f$ $2\times2f$	$2f$ $4g$	$2\times2e$ $4g$	$4g$ $2\times4g$
or: $P12/n1$	**a**–**c**, **b**, **a**+**c**	$\frac{1}{2}(x-z)-\frac{1}{4},y,\frac{1}{2}(x+z)+\frac{1}{4}$; $+(\frac{1}{2},0,\frac{1}{2})$	$2f$	$2f$	$2a$	$2d$	$2b$	$2c$ $4g$	$2e$ $2\times2e$	$2e$ $4g$	$2\times2f$ $4g$	$4g$ $2\times4g$
[2] $C12/m1$ (12)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(0,\frac{1}{2},0)$	$2a;2b$	$4g$	$2c;2d$	$4i$	$4e$	$4h$ $2\times4h$	$4i$ $8j$	$4f$ $2\times4i$	$2\times4g$ $8j$	$8j$ $2\times8j$
[2] $C12/m1$ (12)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z$; $+(0,\frac{1}{2},0)$	$4i$	$4e$	$4i$	$2a;2b$	$4g$	$4f$ $8j$	$2c;2d$ $2\times4h$	$4h$ $2\times4i$	$8j$ $8j$	$2\times4h$ $2\times8j$
[2] $C12/m1$ (12)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z$; $+(0,\frac{1}{2},0)$	$4g$	$2a;2b$	$4h$	$4e$	$4i$	$2c;2d$ $2\times4h$	$4f$ $8j$	$4i$ $8j$	$2\times4g$ $2\times4i$	$8j$ $2\times8j$
[2] $C12/m1$ (12)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z$; $+(0,\frac{1}{2},0)$	$4e$	$4i$	$4f$	$4g$	$2a;2b$	$4i$ $8j$	$4h$ $2\times4h$	$2c;2d$ $8j$	$8j$ $2\times4i$	$2\times4g$ $2\times8j$
[2] $C12/m1$ (12)	2**a**, 2**b**, –**a**+**c**	$\frac{1}{2}(x+z),\frac{1}{2}y,z$; $+(0,\frac{1}{2},0)$	$2a;2b$	$4g$	$4i$	$4i$	$4e$	$4f$ $8j$	$2c;2d$ $2\times4h$	$4h$ $2\times4i$	$2\times4g$ $8j$	$8j$ $2\times8j$
[2] $C12/m1$ (12)	2**a**, 2**b**, –**a**+**c**	$\frac{1}{2}(x+z)+\frac{1}{4},\frac{1}{2}y,z$; $+(0,\frac{1}{2},0)$	$4i$	$4e$	$2c;2d$	$2a;2b$	$4g$	$4h$ $2\times4h$	$4i$ $8j$	$4f$ $2\times4i$	$8j$ $8j$	$2\times4g$ $2\times8j$
[2] $C12/m1$ (12)	2**a**, 2**b**, –**a**+**c**	$\frac{1}{2}(x+z),\frac{1}{2}y+\frac{1}{4},z$; $+(0,\frac{1}{2},0)$	$4g$	$2a;2b$	$4f$	$4e$	$4i$	$4i$ $8j$	$4h$ $2\times4h$	$2c;2d$ $8j$	$2\times4g$ $2\times4i$	$8j$ $2\times8j$
[2] $C12/m1$ (12)	2**a**, 2**b**, –**a**+**c**	$\frac{1}{2}(x+z)+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z$; $+(0,\frac{1}{2},0)$	$4e$	$4i$	$4h$	$4g$	$2a;2b$	$2c;2d$ $2\times4h$	$4f$ $8j$	$4i$ $8j$	$8j$ $2\times4i$	$2\times4g$ $2\times8j$
[2] $A12/m1$ (12)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y,\frac{1}{2}z$; $+(0,\frac{1}{2},0)$;	$2a;2b$	$4g$	$4i$	$2c;2d$	$4h$	$4e$ $8j$	$4i$ $8j$	$4f$ $2\times4i$	$2\times4g$ $8j$	$2\times4h$ $2\times8j$
[2] $A12/m1$ (12)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z$; $+(0,\frac{1}{2},0)$;	$4g$	$2a;2b$	$4e$	$4h$	$2c;2d$	$4i$ $8j$	$4f$ $8j$	$4i$ $8j$	$2\times4g$ $2\times4i$	$2\times4h$ $2\times8j$

* unique axis c

	Axes	Coordinates
I Maximal *translationengleiche* subgroups		
[2] $P11m$		
[2] $P112$		
[2] $P\bar{1}$		
II Maximal *klassengleiche* subgroups		
Enlarged unit cell, non-isomorphic		
[2] $P112/b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$
[2] $P112/b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$
[2] $P112/a$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$
[2] $P112/a$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[2] $P112/a$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), y, z; +(\frac{1}{2}, 0, 0)$
or: $P112/n$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z; +(\frac{1}{2}, \frac{1}{2}, 0)$
[2] $P112/a$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
or: $P112/n$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}(-x+y)-\frac{1}{4}, z; +(\frac{1}{2}, \frac{1}{2}, 0)$
[2] $A112/m$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$
[2] $A112/m$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0, 0, \frac{1}{2})$
[2] $A112/m$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$
[2] $A112/m$	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$
[2] $A112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y), \frac{1}{2}z; +(0, 0, \frac{1}{2})$
[2] $A112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}z; +(0, 0, \frac{1}{2})$
[2] $A112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$
[2] $A112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$
[2] $B112/m$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$
[2] $B112/m$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$

	Axes	Coordinates	Wyckoff positions $1a$	 $1b$ $2i$	 $1c$ $2j$	 $1d$ $2k$	 $1e$ $2l$	 $1f$ $2m$	 $1g$ $2n$	 $1h$ $4o$
[2] $A12/m1$ (12)	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}$; $+(0,\frac{1}{2},0)$	$4i$	$4e$ $8j$	$2a;2b$ $8j$	$4i$ $2\times4g$	$4f$ $2\times4h$	$4g$ $2\times4i$	$2c;2d$ $8j$	$4h$ $2\times8j$
[2] $A12/m1$ (12) (12)	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(0,\frac{1}{2},0)$	$4e$	$4i$ $8j$	$4g$ $8j$	$4f$ $2\times4g$	$4i$ $2\times4h$	$2a;2b$ $8j$	$4h$ $2\times4i$	$2c;2d$ $2\times8j$
[2] $P12_1/m1$ (11)	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0,\frac{1}{2},0)$	$2a$	$2e$ $4f$	$2c$ $4f$	$2b$ $4f$	$2e$ $4f$	$2e$ $4f$	$2d$ $2\times2e$	$2e$ $2\times4f$
[2] $P12_1/m1$ (11)	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0,\frac{1}{2},0)$	$2e$	$2a$ $4f$	$2e$ $4f$	$2e$ $4f$	$2b$ $4f$	$2c$ $2\times2e$	$2e$ $4f$	$2d$ $2\times4f$
Enlarged unit cell, isomorphic										
[2] $P12/m1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0,\frac{1}{2},0)$	$1a;1b$	$2i$ $2\times2i$	$1c;1f$ $2\times2j$	$1d;1e$ $2\times2k$	$2j$ $2\times2l$	$2k$ $2m;2n$	$1g;1h$ $4o$	$2l$ $2\times4o$
[2] $P12/m1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0,\frac{1}{2},0)$	$2i$	$1a;1b$ $2\times2i$	$2k$ $2\times2j$	$2j$ $2\times2k$	$1d;1e$ $2\times2l$	$1c;1f$ $4o$	$2l$ $2m;2n$	$1g;1h$ $2\times4o$
[3] $P12/m1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$	$1a;2i$	$1b;2i$ $3\times2i$	$1c;2k$ $3\times2j$	$1d;2j$ $3\times2k$	$1e;2j$ $3\times2l$	$1f;2k$ $2m;4o$	$1g;2l$ $2n;4o$	$1h;2l$ $3\times4o$
[p] $P12/m1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p=$ prime >2;	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$ $u=1,\dots,p-1$	$1a;\frac{p-1}{2}\times 2i$	$1b;\frac{p-1}{2}\times 2i$ $p\times2i$	$1c;\frac{p-1}{2}\times 2k$ $p\times2j$	$1d;\frac{p-1}{2}\times 2j$ $p\times2k$	$1e;\frac{p-1}{2}\times 2j$ $p\times2l$	$1f;\frac{p-1}{2}\times 2k$ $2m;\frac{p-1}{2}\times 4o$	$1g;\frac{p-1}{2}\times 2l$ $2n;\frac{p-1}{2}\times 4o$	$1h;\frac{p-1}{2}\times 2l$ $p\times4o$
[2] $P12/m1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2},0,0)$	$1a;1d$	$1b;1e$ $2i;2j$	$1c;1g$ $4o$	$2m$ $2k;2l$	$2n$ $4o$	$1f;1h$ $2\times2m$	$2m$ $2\times2n$	$2n$ $2\times4o$
[2] $P12/m1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z$; $+(\frac{1}{2},0,0)$	$2m$	$2n$ $4o$	$2m$ $2i;2j$	$1a;1d$ $4o$	$1b;1e$ $2k;2l$	$2n$ $2\times2m$	$1c;1g$ $2\times2n$	$1f;1h$ $2\times4o$
[2] $P12/m1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, \frac{1}{2}(x+z)$; $+(\frac{1}{2},0,\frac{1}{2})$	$1a;1g$	$1b;1h$ $2i;2l$	$2m$ $4o$	$2m$ $4o$	$2n$ $2j;2k$	$2n$ $2\times2m$	$1c;1d$ $2\times2n$	$1e;1f$ $2\times4o$
[2] $P12/m1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z)+\frac{1}{4}, y,$ $\frac{1}{2}(x+z)+\frac{1}{4}$; $+(\frac{1}{2},0,\frac{1}{2})$	$2m$	$2n$ $4o$	$1c;1d$ $2i;2l$	$1a;1g$ $2j;2k$	$1b;1h$ $4o$	$1e;1f$ $2\times2m$	$2m$ $2\times2n$	$2n$ $2\times4o$
[2] $P12/m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a;1c$	$1b;1f$ $2i;2k$	$2m$ $2j;2l$	$1d;1g$ $4o$	$1e;1h$ $4o$	$2n$ $2\times2m$	$2m$ $2\times2n$	$2n$ $2\times4o$
[2] $P12/m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2m$	$2n$ $4o$	$1a;1c$ $4o$	$2m$ $2i;2k$	$2n$ $2j;2l$	$1b;1f$ $2\times2m$	$1d;1g$ $2\times2n$	$1e;1h$ $2\times4o$
[3] $P12/m1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$	$1a;2m$	$1b;2n$ $2i;4o$	$1c;2m$ $2j;4o$	$1d;2m$ $2k;4o$	$1e;2n$ $2l;4o$	$1f;2n$ $3\times2m$	$1g;2m$ $3\times2n$	$1h;2n$ $3\times4o$
[3] $P12/m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a;2m$	$1b;2n$ $2i;4o$	$1c;2m$ $2j;4o$	$1d;2m$ $2k;4o$	$1e;2n$ $2l;4o$	$1f;2n$ $3\times2m$	$1g;2m$ $3\times2n$	$1h;2n$ $3\times4o$
[3] $P12/m1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(x+z)$; $\pm(0,0,\frac{1}{3})$	$1a;2m$	$1b;2n$ $2i;4o$	$1c;2m$ $2l;4o$	$1g;2m$ $2k;4o$	$1h;2n$ $2j;4o$	$1f;2n$ $3\times2m$	$1d;2m$ $3\times2n$	$1e;2n$ $3\times4o$
[3] $P12/m1$	$\mathbf{a}+\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(-x+z)$; $\pm(0,0,\frac{1}{3})$	$1a;2m$	$1b;2n$ $2i;4o$	$1c;2m$ $2l;4o$	$1g;2m$ $2k;4o$	$1h;2n$ $2j;4o$	$1f;2n$ $3\times2m$	$1d;2m$ $3\times2n$	$1e;2n$ $3\times4o$
[p] $P12/m1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$ $p=$prime >2;	$\frac{1}{p}x, y, z$; $+(\frac{u}{p},0,0)$ $u=1,\dots,p-1$	$1a;\frac{p-1}{2}\times 2m$	$1b;\frac{p-1}{2}\times 2n$ $2i;\frac{p-1}{2}\times 4o$	$1c;\frac{p-1}{2}\times 2m$ $2j;\frac{p-1}{2}\times 4o$	$1d;\frac{p-1}{2}\times 2m$ $2k;\frac{p-1}{2}\times 4o$	$1e;\frac{p-1}{2}\times 2n$ $2l;\frac{p-1}{2}\times 4o$	$1f;\frac{p-1}{2}\times 2n$ $p\times2m$	$1g;\frac{p-1}{2}\times 2m$ $p\times2n$	$1h;\frac{p-1}{2}\times 2n$ $p\times4o$
[p] $P12/m1$	$\mathbf{a}+q\mathbf{c}, \mathbf{b}, p\mathbf{c}$ $p=$prime >2; $u=1,\dots,p-1$ $-\frac{1}{2}(p-1)\leq q\leq\frac{1}{2}(p-1)$	$x, y, \frac{1}{p}(-qx+z)$; $+(0,0,\frac{u}{p})$	$1a;\frac{p-1}{2}\times 2m$	$1b;\frac{p-1}{2}\times 2n$ $2i;\frac{p-1}{2}\times 4o$	$1c;\frac{p-1}{2}\times 2m$ $2j(l^*)$; $\frac{p-1}{2}\times 4o$	$1d(g^*)$; $\frac{p-1}{2}\times 2m$ $2k;\frac{p-1}{2}\times 4o$	$1e(h^*)$; $\frac{p-1}{2}\times 2n$ $2l(j^*)$; $\frac{p-1}{2}\times 4o$	$1f;\frac{p-1}{2}\times 2n$ $p\times2m$	$1g(d^*)$; $\frac{p-1}{2}\times 2m$ $p\times2n$	$1h(e^*)$; $\frac{p-1}{2}\times 2n$ $p\times4o$

* $q=2n+1$

	Axes	Coordinates
[2] $B112/m$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$
[2] $B112/m$	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$
[2] $P112_1/m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$
[2] $P112_1/m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$

Enlarged unit cell, isomorphic

[2] $P112/m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$
[2] $P112/m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$
[3] $P112/m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$
[p] $P112/m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p = $ prime > 2; $u = 1, \ldots, p-1$
[2] $P112/m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z$; $+(0,\frac{1}{2},0)$
[2] $P112/m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z$; $+(0,\frac{1}{2},0)$
[2] $P112/m$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$
[2] $P112/m$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}(-x+y)+\frac{1}{4}, z$; $+(\frac{1}{2},\frac{1}{2},0)$
[2] $P112/m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z$; $+(\frac{1}{2},0,0)$
[2] $P112/m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z$; $+(\frac{1}{2},0,0)$
[3] $P112/m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$
[3] $P112/m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$
[3] $P112/m$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), y, z$; $\pm(\frac{1}{3},0,0)$
[3] $P112/m$	$3\mathbf{a}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x-y), y, z$; $\pm(\frac{1}{3},0,0)$
[p] $P112/m$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$ $p = $prime > 2; $u = 1, \ldots, p-1$
[p] $P112/m$	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(x-qy), y, z$; $+(\frac{u}{p},0,0)$ $p = $prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 11, pp. 456–457.

$P2_1/m$ No. 11 $P12_1/m1$ C_{2h}^2

UNIQUE AXIS b

	Axes	Coordinates	Wyckoff positions 2a	2b	2c	2d	2e	4f
I Maximal *translationengleiche* subgroups								
[2] $P1m1$ (6)		$x,y+\frac{1}{4},z$	$2c$	$2c$	$2c$	$2c$	$1a;1b$	$2\times2c$
[2] $P12_11$ (4)			$2a$	$2a$	$2a$	$2a$	$2a$	$2\times2a$
[2] $P\bar{1}$ (2)			$1a;1c$	$1d;1e$	$1b;1g$	$1f;1h$	$2i$	$2\times2i$
			$1a;1b$	$1c;1g$	$1d;1f$	$1e;1h$	$2i$	$2\times2i$ ⇒
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P12_1/a1$ (14)	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2a;2c$	$4e$	$2b;2d$	$4e$	$4e$	$2\times4e$
[2] $P12_1/a1$ (14)	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4e$	$2a;2c$	$4e$	$2b;2d$	$4e$	$2\times4e$
[2] $P12_1/c1$ (14)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a;2c$	$2b;2d$	$4e$	$4e$	$4e$	$2\times4e$
[2] $P12_1/c1$ (14)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4e$	$4e$	$2a;2c$	$2b;2d$	$4e$	$2\times4e$
[2] $P12_1/c1$ (14)	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}(x+z);\ +(0,0,\frac{1}{2})$	$2a;2c$	$4e$	$4e$	$2b;2d$	$4e$	$2\times4e$
[2] $P12_1/c1$ (14)	$\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}(x+z)+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4e$	$2b;2d$	$2a;2c$	$4e$	$4e$	$2\times4e$
Enlarged unit cell, isomorphic								
[3] $P12_1/m1$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$2a;4f$	$2b;4f$	$2c;4f$	$2d;4f$	$2e;4f$	$3\times4f$
[p] $P12_1/m1$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$2a;\frac{p-1}{2}\times4f$	$2b;\frac{p-1}{2}\times4f$	$2c;\frac{p-1}{2}\times4f$	$2d;\frac{p-1}{2}\times4f$	$2e;\frac{p-1}{2}\times4f$	$p\times4f$
	$p=$ prime >2; $u=1,\ldots,p-1$							
[2] $P12_1/m1$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2a;2b$	$4f$	$2c;2d$	$4f$	$2\times2e$	$2\times4f$
[2] $P12_1/m1$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4f$	$2a;2b$	$4f$	$2c;2d$	$2\times2e$	$2\times4f$
[2] $P12_1/m1$	$\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z),y,\frac{1}{2}(x+z);+(\frac{1}{2},0,\frac{1}{2})$	$2a;2d$	$4f$	$4f$	$2b;2c$	$2\times2e$	$2\times4f$
	or: $\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}(x+z);+(0,0,\frac{1}{2})$	$2a;2c$	$4f$	$4f$	$2b;2d$	$2\times2e$	$2\times4f$
[2] $P12_1/m1$	$\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z)+\frac{1}{4},y,\frac{1}{2}(x+z)+\frac{1}{4};$ $+(\frac{1}{2},0,\frac{1}{2})$	$4f$	$2a;2d$	$2b;2c$	$4f$	$2\times2e$	$2\times4f$
	or: $\mathbf{a}-\mathbf{c},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}(x+z)+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	$4f$	$2b;2d$	$2a;2c$	$4f$	$2\times2e$	$2\times4f$
[2] $P12_1/m1$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a;2c$	$2b;2d$	$4f$	$4f$	$2\times2e$	$2\times4f$
[2] $P12_1/m1$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4f$	$4f$	$2a;2c$	$2b;2d$	$2\times2e$	$2\times4f$
[3] $P12_1/m1$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4f$	$2b;4f$	$2c;4f$	$2d;4f$	$3\times2e$	$3\times4f$
[3] $P12_1/m1$	$3\mathbf{a},\mathbf{b},-\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z),y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4f$	$2b;4f$	$2d;4f$	$2c;4f$	$3\times2e$	$3\times4f$
[3] $P12_1/m1$	$3\mathbf{a},\mathbf{b},\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z),y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4f$	$2b;4f$	$2d;4f$	$2c;4f$	$3\times2e$	$3\times4f$
[3] $P12_1/m1$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4f$	$2b;4f$	$2c;4f$	$2d;4f$	$3\times2e$	$3\times4f$
[p] $P12_1/m1$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4f$	$2b;\frac{p-1}{2}\times4f$	$2c;\frac{p-1}{2}\times4f$	$2d;\frac{p-1}{2}\times4f$	$p\times2e$	$p\times4f$
	$p=$ prime >2; $u=1,\ldots,p-1$							
[p] $P12_1/m1$	$p\mathbf{a},\mathbf{b},q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz),y,z;\ +(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}\times4f$	$2b;\frac{p-1}{2}\times4f$	$2c(d^*);$ $\frac{p-1}{2}\times4f$	$2d(c^*);$ $\frac{p-1}{2}\times4f$	$p\times2e$	$p\times4f$
	$p=$ prime >2; $u=1,\ldots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$							

$^*\,q=2n+1$

	Axes	Coordinates
I Maximal *translationengleiche* subgroups		
[2] $P11m$		$x, y, z+\frac{1}{4}$
[2] $P112_1$		
[2] $P\bar{1}$		
II Maximal *klassengleiche* subgroups		
Enlarged unit cell, non-isomorphic		
[2] $P112_1/b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$
[2] $P112_1/b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z;\ +(0, \frac{1}{2}, 0)$
[2] $P112_1/a$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$
[2] $P112_1/a$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$
[2] $P112_1/a$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), y, z;\ +(\frac{1}{2}, 0, 0)$
[2] $P112_1/a$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$
Enlarged unit cell, isomorphic		
[3] $P112_1/m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$
[p] $P112_1/m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0, 0, \frac{u}{p})$
	$p =$ prime > 2; $u = 1, \ldots, p-1$	
[2] $P112_1/m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$
[2] $P112_1/m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z;\ +(0, \frac{1}{2}, 0)$
[2] $P112_1/m$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z; +(\frac{1}{2}, \frac{1}{2}, 0)$
	or: $2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), y, z; +(\frac{1}{2}, 0, 0)$
[2] $P112_1/m$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}(-x+y)+\frac{1}{4}, z; +(\frac{1}{2}, \frac{1}{2}, 0)$
	or: $2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$
[2] $P112_1/m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$
[2] $P112_1/m$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$
[3] $P112_1/m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$
[3] $P112_1/m$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z;\ \pm(0, \frac{1}{3}, 0)$
[3] $P112_1/m$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z;\ \pm(0, \frac{1}{3}, 0)$
[3] $P112_1/m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$
[p] $P112_1/m$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$
	$p =$ prime > 2; $u = 1, \ldots, p-1$	
[p] $P112_1/m$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-qx+y), z;\ +(0, \frac{u}{p}, 0)$
	$p =$ prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

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$C2/m$ No. 12 $C12/m1$ C_{2h}^{3}

UNIQUE AXIS b, CELL CHOICE 1

	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$4i$	$8j$	
I Maximal *translationengleiche* subgroups													
[2] $C1m1$ (8)			$2a$	$2a$	$2a$	$2a$	$4b$	$4b$	$4b$	$4b$	$2\times2a$	$2\times4b$	
[2] $C121$(5)			$2a$	$2a$	$2b$	$2b$	$4c$	$4c$	$2\times2a$	$2\times2b$	$4c$	$2\times4c$	
[2] $P\bar{1}$ (2)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$,	$2x, x+y, z$	$1a$	$1c$	$1b$	$1g$	$1d; 1e$	$1f; 1h$	$2i$	$2i$	$2i$	$2\times2i$	
	$\mathbf{b}$, $\mathbf{c}$		$1a$	$1c$	$1e$	$1d$	$1b; 1g$	$1f; 1h$	$2i$	$2i$	$2i$	$2\times2i$	⇒
			$1a$	$1f$	$1d$	$1b$	$1c; 1h$	$1e; 1g$	$2i$	$2i$	$2i$	$2\times2i$	⇒
II Maximal *klassengleiche* subgroups													
Loss of centring translations													
[2] $P12_1/a1$ (14)			$2a$	$2c$	$2d$	$2b$	$4e$	$4e$	$4e$	$4e$	$4e$	$2\times4e$	
[2] $P12/a1$ (13)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$2e$	$2e$	$2f$	$2f$	$2a; 2c$	$2b; 2d$	$2\times2e$	$2\times2f$	$4g$	$2\times4g$	
[2] $P12_1/m1$ (11)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$2e$	$2e$	$2e$	$2e$	$2a; 2b$	$2c; 2d$	$4f$	$4f$	$2\times2e$	$2\times4f$	
			$2e$	$2e$	$2e$	$2e$	$2a; 2c$	$2b; 2d$	$4f$	$4f$	$2\times2e$	$2\times4f$	⇒
			$2e$	$2e$	$2e$	$2e$	$2a; 2d$	$2b; 2c$	$4f$	$4f$	$2\times2e$	$2\times4f$	⇒
[2] $P12/m1$ (10)			$1a; 1e$	$1b; 1d$	$1c; 1h$	$1f; 1g$	$4o$	$4o$	$2i; 2j$	$2k; 2l$	$2m; 2n$	$2\times4o$	
			$1a; 1f$	$1b; 1c$	$1e; 1g$	$1d; 1h$	$4o$	$4o$	$2i; 2k$	$2j; 2l$	$2m; 2n$	$2\times4o$	⇒
			$1a; 1h$	$1b; 1g$	$1d; 1f$	$1c; 1e$	$4o$	$4o$	$2i; 2l$	$2j; 2k$	$2m; 2n$	$2\times4o$	⇒
Enlarged unit cell, non-isomorphic													
[2] $C12/c1$ (15)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4a$	$4b$	$4e$	$4e$	$4c; 4d$	$8f$	$8f$	$2\times4e$	$8f$	$2\times8f$	
[2] $C12/c1$ (15)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4e$	$4e$	$4a$	$4b$	$8f$	$4c; 4d$	$2\times4e$	$8f$	$8f$	$2\times8f$	
[2] $C12/c1$ (15) or: $I12/a1$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 2\mathbf{c}$ or: $2\mathbf{c}, -\mathbf{b}, \mathbf{a}$	$x, y, x+\frac{1}{2}z; +(0,0,\frac{1}{2})$ or: $\frac{1}{2}z, -y, x; +(\frac{1}{2},0,0)$	$4a$	$4b$	$4e$	$4e$	$8f$	$4c; 4d$	$8f$	$2\times4e$	$8f$	$2\times8f$	
[2] $C12/c1$ (15) or: $I12/a1$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 2\mathbf{c}$ or: $2\mathbf{c}, -\mathbf{b}, \mathbf{a}$	$x, y, x+\frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$ or: $\frac{1}{2}z+\frac{1}{4}, -y, x; +(\frac{1}{2},0,0)$	$4e$	$4e$	$4a$	$4b$	$4c; 4d$	$8f$	$2\times4e$	$8f$	$8f$	$2\times8f$	
Enlarged unit cell, isomorphic													
[3] $C12/m1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$	$2a; 4g$	$2b; 4g$	$2c; 4h$	$2d; 4h$	$4e; 8j$	$4f; 8j$	$3\times4g$	$3\times4h$	$4i; 8j$	$3\times8j$	
[p] $C12/m1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0,\frac{u}{p},0)$ p = prime > 2; $u = 1,\ldots,p-1$	$2a; \frac{p-1}{2}\times 4g$	$2b; \frac{p-1}{2}\times 4g$	$2c; \frac{p-1}{2}\times4h$	$2d; \frac{p-1}{2}\times4h$	$4e; \frac{p-1}{2}\times8j$	$4f; \frac{p-1}{2}\times8j$	$p\times4g$	$p\times4h$	$4i; \frac{p-1}{2}\times8j$	$p\times8j$	
[2] $C12/m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a; 2c(d^*)$	$2b; 2d(c^*)$	$4i$	$4i$	$4e; 4f$	$8j$	$4g; 4h$	$8j$	$2\times4i$	$2\times8j$	
[2] $C12/m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4i$	$4i$	$2a(b^*)$; $2c$	$2b(a^*)$; $2d$	$8j$	$4e; 4f$	$8j$	$4g; 4h$	$2\times4i$	$2\times8j$	
[2] $I12/m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a; 2d$	$2b; 2c$	$4i$	$4i$	$8j$	$4e; 4f$	$4g; 4h$	$8j$	$2\times4i$	$2\times8j$	
[2] $I12/m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4i$	$4i$	$2a; 2d$	$2b; 2c$	$4e; 4f$	$8j$	$8j$	$4g; 4h$	$2\times4i$	$2\times8j$	
[3] $C12/m1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$	$2a; 4i$	$2b; 4i$	$2c; 4i$	$2d; 4i$	$4e(f^\dagger)$; $8j$	$4f(e^\dagger)$; $8j$	$4g; 8j$	$4h; 8j$	$3\times4i$	$3\times8j$	
[3] $C12/m1$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z; \pm(\frac{1}{3},0,0)$	$2a; 4i$	$2b; 4i$	$2d(c^\dagger)$; $4i$	$2c(d^\dagger)$; $4i$	$4e; 8j$	$4f; 8j$	$4g; 8j$	$4h; 8j$	$3\times4i$	$3\times8j$	
[3] $C12/m1$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z; \pm(\frac{1}{3},0,0)$	$2a; 4i$	$2b; 4i$	$2d(c^{\dagger\dagger})$; $4i$	$2c(d^{\dagger\dagger})$; $4i$	$4e(f^\dagger)$; $8j$	$4f(e^\dagger)$; $8j$	$4g; 8j$	$4h; 8j$	$3\times4i$	$3\times8j$	
[3] $C12/m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$2a; 4i$	$2b; 4i$	$2c; 4i$	$2d; 4i$	$4e; 8j$	$4f; 8j$	$4g; 8j$	$4h; 8j$	$3\times4i$	$3\times8j$	
[p] $C12/m1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$ p = prime > 2; $u = 1,\ldots,p-1$	$2a; \frac{p-1}{2}\times 4i$	$2b; \frac{p-1}{2}\times 4i$	$2c; \frac{p-1}{2}\times4i$	$2d; \frac{p-1}{2}\times4i$	$4e(f^\ddagger)$; $\frac{p-1}{2}\times8j$	$4f(e^\ddagger)$; $\frac{p-1}{2}\times8j$	$4g; \frac{p-1}{2}\times8j$	$4h; \frac{p-1}{2}\times8j$	$p\times4i$	$p\times8j$	
[p] $C12/m1$	$p\mathbf{a}, \mathbf{b}, q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z; +(\frac{u}{p},0,0)$ p = prime > 2; $u = 1,\ldots,p-1$ $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	$2a; \frac{p-1}{2}\times 4i$	$2b; \frac{p-1}{2}\times 4i$	$2c(d^\S)$; $\frac{p-1}{2}\times4i$	$2d(c^\S)$; $\frac{p-1}{2}\times4i$	$4e(f^\sharp)$; $\frac{p-1}{2}\times8j$	$4f(e^\sharp)$; $\frac{p-1}{2}\times8j$	$4g; \frac{p-1}{2}\times8j$	$4h; \frac{p-1}{2}\times8j$	$p\times4i$	$p\times8j$	

* cell choice 2 ($A12/m1$)

† cell choice 3 ($I12/m1$)

†† cell choices 2 or 3

§ cell choices 1 or 2 and $q = 2n+1$

‡ cell choice 3 ($I12/m1$) and $p = 4n-1$

$^\sharp$ cell choice 3 ($I12/m1$) and $p+2q = 4n-1$

		Axes	Coordinates		Axes	Coordinates
I	**Maximal *translationengleiche* subgroups**					
[2]	$A1m1$			$I1m1$		
[2]	$A121$			$I121$		
[2]	$P\bar{1}$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x, y+z, 2z$	$P\bar{1}$	$\mathbf{a}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c}), \mathbf{c}$	$x+y, 2y, y+z$
II	**Maximal *klassengleiche* subgroups**					
	Loss of centring translations					
[2]	$P12_1/c1$			$P12_1/n1$		
[2]	$P12/c1$		$x, y+\frac{1}{4}, z+\frac{1}{4}$	$P12/n1$		$x-\frac{1}{4}, y+\frac{1}{4}, z-\frac{1}{4}$
[2]	$P12_1/m1$		$x, y+\frac{1}{4}, z+\frac{1}{4}$	$P12_1/m1$		$x-\frac{1}{4}, y+\frac{1}{4}, z-\frac{1}{4}$
[2]	$P12/m1$			$P12/m1$		
	Enlarged unit cell, non-isomorphic					
[2]	$A12/n1$	$2\mathbf{a}+\mathbf{c}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, -\frac{1}{2}x+z;\ +(\frac{1}{2}, 0, \frac{1}{2})$	$I12/a1$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), y, z;\ +(\frac{1}{2}, 0, 0)$
[2]	$A12/n1$	$2\mathbf{a}+\mathbf{c}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, -\frac{1}{2}x+z-\frac{1}{4};\ +(\frac{1}{2}, 0, \frac{1}{2})$	$I12/a1$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z)+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$
[2]	$I12/a1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$I12/a1$	$2\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z), y, z;\ +(\frac{1}{2}, 0, 0)$
				or: $C12/c1$	$-\mathbf{a}+\mathbf{c}, -\mathbf{b}, 2\mathbf{a}$	$z, -y, \frac{1}{2}(x+z);\ +(0, 0, \frac{1}{2})$
[2]	$I12/a1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, z+\frac{1}{2};\ +(\frac{1}{2}, 0, 0)$	$I12/a1$	$2\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x-z)+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$
				or: $C12/c1$	$-\mathbf{a}+\mathbf{c}, -\mathbf{b}, 2\mathbf{a}$	$z, -y, \frac{1}{2}(x+z)+\frac{1}{4};\ +(0, 0, \frac{1}{2})$
	Enlarged unit cell, isomorphic					
[3]	$A12/m1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	$I12/m1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$
[p]	$A12/m1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$	$I12/m1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$
		p = prime > 2; $u = 1, \ldots, p-1$			p = prime > 2; $u = 1, \ldots, p-1$	
[2]	$A12/m1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$I12/m1$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), y, z;\ +(\frac{1}{2}, 0, 0)$
[2]	$A12/m1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$I12/m1$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z)+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$
[2]	$C12/m1$	$2\mathbf{a}+\mathbf{c}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, -\frac{1}{2}x+z;\ +(\frac{1}{2}, 0, \frac{1}{2})$	$A12/m1$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z), y, z;\ +(\frac{1}{2}, 0, 0)$
[2]	$C12/m1$	$2\mathbf{a}+\mathbf{c}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, -\frac{1}{2}x+z-\frac{1}{4};\ +(\frac{1}{2}, 0, \frac{1}{2})$	$A12/m1$	$2\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{2}(x+z)+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$
[3]	$A12/m1$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(2x+z);\ \pm(0, 0, \frac{1}{3})$	$I12/m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$
[3]	$A12/m1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(x+z);\ \pm(0, 0, \frac{1}{3})$	$I12/m1$	$3\mathbf{a}, \mathbf{b}, 2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-2z), y, z;\ \pm(\frac{1}{3}, 0, 0)$
[3]	$A12/m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	$I12/m1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$
[3]	$A12/m1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	$I12/m1$	$3\mathbf{a}, \mathbf{b}, -2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+2z), y, z;\ \pm(\frac{1}{3}, 0, 0)$
[p]	$A12/m1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$	$I12/m1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z;\ \pm(\frac{u}{p}, 0, 0)$
		p = prime > 2; $u = 1, \ldots, p-1$			p = prime > 2; $u = 1, \ldots, p-1$	
[p]	$A12/m1$	$\mathbf{a}+q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}(-qx+z);\ +(0, 0, \frac{u}{p})$	$I12/m1$	$\mathbf{a}+2q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}(-2qx+z);\ +(0, 0, \frac{u}{p})$
		$-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$			$-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

	Axes	Coordinates	Wyckoff positions 2a	2b	2c	2d	4e	4f	4g	4h	4i	8j	
I Maximal *translationengleiche* subgroups													
[2] $A11m$ (8)			2a	2a	2a	2a	4b	4b	4b	4b	2×2a	2×4b	
[2] $A112$ (5)			2a	2a	2b	2b	4c	4c	2×2a	2×2b	4c	2×4c	
[2] $P\bar{1}$ (2)	**a**, $\frac{1}{2}$(**b**−**c**), **c**	$x, 2y, y+z$	1a	1b	1d	1f	1c; 1g	1e; 1h	2i	2i	2i	2×2i	
			1a	1b	1g	1c	1d; 1f	1e; 1h	2i	2i	2i	2×2i	⇒
			1a	1e	1c	1d	1b; 1h	1f; 1g	2i	2i	2i	2×2i	⇒
II Maximal *klassengleiche* subgroups													
Loss of centring translations													
[2] $P112_1/b$ (14)			2a	2c	2d	2b	4e	4e	4e	4e	4e	2×4e	
[2] $P112/b$ (13)		$x, y+\frac{1}{4}, z+\frac{1}{4}$	2e	2e	2f	2f	2a; 2c	2b; 2d	2×2e	2×2f	4g	2×4g	
[2] $P112_1/m$ (11)		$x, y+\frac{1}{4}, z+\frac{1}{4}$	2e	2e	2e	2e	2a; 2b	2c; 2d	4f	4f	2×2e	2×4f	
			2e	2e	2e	2e	2a; 2c	2b; 2d	4f	4f	2×2e	2×4f	⇒
			2e	2e	2e	2e	2a; 2d	2b; 2c	4f	4f	2×2e	2×4f	⇒
[2] $P112/m$ (10)			1a; 1e	1b; 1d	1c; 1h	1f; 1g	4o	4o	2i; 2j	2k; 2l	2m; 2n	2×4o	
			1a; 1f	1b; 1c	1e; 1g	1d; 1h	4o	4o	2i; 2k	2j; 2l	2m; 2n	2×4o	⇒
			1a; 1h	1b; 1g	1d; 1f	1c; 1e	4o	4o	2i; 2l	2j; 2k	2m; 2n	2×4o	⇒
Enlarged unit cell, non-isomorphic													
[2] $A112/a$ (15)	2**a**, **b**, **c**	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$	4a	4b	4e	4e	4c; 4d	8f	8f	2×4e	8f	2×8f	
[2] $A112/a$ (15)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	4e	4e	4a	4b	8f	4c; 4d	2×4e	8f	8f	2×8f	
[2] $A112/a$ (15) or: $I112/b$	2**a**,−2**a**+**b**, **c**; **b**, 2**a**, −**c**	$\frac{1}{2}x+y, y, z; +(\frac{1}{2}, 0, 0)$; $y, \frac{1}{2}x, -z; +(0, \frac{1}{2}, 0)$	4a	4b	4e	4e	8f	4c; 4d	8f	2×4e	8f	2×8f	
[2] $A112/a$ (15) or: $I112/b$	2**a**,−2**a**+**b**, **c**; **b**, 2**a**, −**c**	$\frac{1}{2}x+y+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$; $y, \frac{1}{2}x+\frac{1}{4}, -z; +(0, \frac{1}{2}, 0)$	4e	4e	4a	4b	4c; 4d	8f	2×4e	8f	8f	2×8f	
Enlarged unit cell, isomorphic													
[3] $A112/m$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	2a; 4g	2b; 4g	2c; 4h	2d; 4h	4e; 8j	4f; 8j	3×4g	3×4h	4i; 8j	3×8j	
[p] $A112/m$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$; p = prime > 2; $u = 1, \ldots, p-1$	2a; $\frac{p-1}{2}$×4g	2b; $\frac{p-1}{2}$×4g	2c; $\frac{p-1}{2}$×4h	2d; $\frac{p-1}{2}$×4h	4e; $\frac{p-1}{2}$×8j	4f; $\frac{p-1}{2}$×8j	p×4g	p×4h	4i; $\frac{p-1}{2}$×8j	p×8j	
[2] $A112/m$	2**a**, **b**, **c**	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$	2a; 2c(d*)	2b; 2d(c*)	4i	4i	4e; 4f	8j	4g; 4h	8j	2×4i	2×8j	
[2] $A112/m$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	4i	4i	2a(b*); 2c	2b(a*); 2d	8j	4e; 4f	8j	4g; 4h	2×4i	2×8j	
[2] $I112/m$	2**a**, **b**, **c**	$\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$	2a; 2d	2b; 2c	4i	4i	8j	4e; 4f	4g; 4h	8j	2×4i	2×8j	
[2] $I112/m$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$	4i	4i	2a; 2d	2b; 2c	4e; 4f	8j	8j	4g; 4h	2×4i	2×8j	
[3] $A112/m$	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	2a; 4i	2b; 4i	2c; 4i	2d; 4i	4e(f†); 8j	4f(e†); 8j	4g; 8j	4h; 8j	3×4i	3×8j	
[3] $A112/m$	**a**−**b**, 3**b**, **c**	$x, \frac{1}{3}(x+y), z; \pm(0, \frac{1}{3}, 0)$	2a; 4i	2b; 4i	2d(c†); 4i	2c(d†); 4i	4e; 8j	4f; 8j	4g; 8j	4h; 8j	3×4i	3×8j	
[3] $A112/m$	**a**+**b**, 3**b**, **c**	$x, \frac{1}{3}(-x+y), z; \pm(0, \frac{1}{3}, 0)$	2a; 4i	2b; 4i	2d(c††); 4i	2c(d††); 4i	4e(f†); 8j	4f(e†); 8j	4g; 8j	4h; 8j	3×4i	3×8j	
[3] $A112/m$	3**a**, **b**, **c**	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	2a; 4i	2b; 4i	2c; 4i	2d; 4i	4e; 8j	4f; 8j	4g; 8j	4h; 8j	3×4i	3×8j	
[p] $A112/m$	p**a**, **b**, **c**	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$; p = prime > 2; $u = 1, \ldots, p-1$	2a; $\frac{p-1}{2}$×4i	2b; $\frac{p-1}{2}$×4i	2c; $\frac{p-1}{2}$×4i	2d; $\frac{p-1}{2}$×4i	4e(f‡); $\frac{p-1}{2}$×8j	4f(e‡); $\frac{p-1}{2}$×8j	4g; $\frac{p-1}{2}$×8j	4h; $\frac{p-1}{2}$×8j	p×4i	p×8j	
[p] $A112/m$	**a**+q**b**, p**b**, **c**	$x, \frac{1}{p}(-qx+y), z; +(0, \frac{u}{p}, 0)$; p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	2a; $\frac{p-1}{2}$×4i	2b; $\frac{p-1}{2}$×4i	2c(d§); $\frac{p-1}{2}$×4i	2d(c§); $\frac{p-1}{2}$×4i	4e(f♯); $\frac{p-1}{2}$×8j	4f(e♯); $\frac{p-1}{2}$×8j	4g; $\frac{p-1}{2}$×8j	4h; $\frac{p-1}{2}$×8j	p×4i	p×8j	

* cell choice 2 ($B112/m$)

† cell choice 3 ($I112/m$)

†† cell choices 2 or 3

§ cell choices 1 or 2 and $q = 2n+1$

‡ cell choice 3 ($I112/m$) and $p = 4n-1$

♯ cell choice 3 ($I112/m$) and $p+2q = 4n-1$

	Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups					
[2] $B11m$			$I11m$		
[2] $B112$			$I112$		
[2] $P\bar{1}$	$\frac{1}{2}(\mathbf{a}-\mathbf{c}), \mathbf{b}, \mathbf{c}$	$2x, y, x+z$			
			$P\bar{1}$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$x+y, y+z, 2z$
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $P112_1/a$			$P112_1/n$		
[2] $P112/a$		$x+\frac{1}{4}, y, z+\frac{1}{4}$	$P112/n$		$x-\frac{1}{4}, y-\frac{1}{4}, z+\frac{1}{4}$
[2] $P112_1/m$		$x+\frac{1}{4}, y, z+\frac{1}{4}$			
			$P112_1/m$		$x-\frac{1}{4}, y-\frac{1}{4}, z+\frac{1}{4}$
[2] $P112/m$					
			$P112/m$		
Enlarged unit cell, non-isomorphic					
[2] $B112/n$	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$I112/b$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z; +(0, \frac{1}{2}, 0)$
[2] $B112/n$	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y-\frac{1}{4}, \frac{1}{2}y-\frac{1}{4}, z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$I112/b$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y)+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$
[2] $I112/b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$	$I112/b$	$\mathbf{a}+\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(-x+y), z; +(0, \frac{1}{2}, 0)$
			or: $A112/a$	$2\mathbf{b}, \mathbf{a}-\mathbf{b}, -\mathbf{c}$	$\frac{1}{2}(x+y), x, -z; +(\frac{1}{2}, 0, 0)$
[2] $I112/b$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x+\frac{1}{2}, \frac{1}{2}y-\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$	$I112/b$	$\mathbf{a}+\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(-x+y)+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$
			or: $A112/a$	$2\mathbf{b}, \mathbf{a}-\mathbf{b}, -\mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, x, -z; +(\frac{1}{2}, 0, 0)$
Enlarged unit cell, isomorphic					
[3] $B112/m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$I112/m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$
[p] $B112/m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$I112/m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$
	$p = \text{prime} > 2;\ u = 1, \dots, p-1$			$p = \text{prime} > 2;\ u = 1, \dots, p-1$	
[2] $B112/m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$	$I112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z; +(0, \frac{1}{2}, 0)$
[2] $B112/m$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y-\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$	$I112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y)+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$
[2] $A112/m$	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$B112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y), z; +(0, \frac{1}{2}, 0)$
[2] $A112/m$	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y-\frac{1}{4}, \frac{1}{2}y-\frac{1}{4}, z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$B112/m$	$\mathbf{a}-\mathbf{b}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}(x+y)+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$
[3] $B112/m$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+2y), y, z; \pm(\frac{1}{3}, 0, 0)$	$I112/m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$
[3] $B112/m$	$3\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), y, z; \pm(\frac{1}{3}, 0, 0)$	$I112/m$	$\mathbf{a}+2\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-2x+y), z; \pm(0, \frac{1}{3}, 0)$
[3] $B112/m$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$I112/m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$
[3] $B112/m$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$I112/m$	$\mathbf{a}-2\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(2x+y), z; \pm(0, \frac{1}{3}, 0)$
[p] $B112/m$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$I112/m$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; \pm(0, \frac{u}{p}, 0)$
	$p = \text{prime} > 2;\ u = 1, \dots, p-1$			$p = \text{prime} > 2;\ u = 1, \dots, p-1$	
[p] $B112/m$	$p\mathbf{a}, q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(x-qy), y, z; +(\frac{u}{p}, 0, 0)$	$I112/m$	$p\mathbf{a}, 2q\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{p}(x-2qy), y, z; +(\frac{u}{p}, 0, 0)$
	$-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$			$-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 13, pp. 462–465.

$P2/c$ No. 13 $P12/c1$ C_{2h}^{4}

UNIQUE AXIS b, CELL CHOICE 1

	Axes	Coordinates	Wyckoff positions 2a	2b	2c	2d	2e	2f	4g	
I Maximal *translationengleiche* subgroups										
[2] $P1c1$ (7)			2a	2a	2a	2a	2a	2a	2×2a	
[2] $P121$ (3)		$x,y,z+\frac{1}{4}$	2e	2e	2e	2e	1a;1b	1c;1d	2×2e	
[2] $P\bar{1}$ (2)			1a;1b	1e;1h	1c;1g	1d;1f	2i	2i	2×2i	
			1a;1f	1e;1g	1c;1h	1b;1d	2i	2i	2×2i	⇒
			1a;1d	1g;1h	1c;1e	1b;1f	2i	2i	2×2i	⟹
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $C12/c1$ (15)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	4a;4b	4c;4d	8f	8f	2×4e	8f	2×8f	
[2] $C12/c1$ (15)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	8f	8f	4c;4d	4a;4b	8f	2×4e	2×8f	
[2] $C12/c1$ (15)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	8f	8f	4a;4b	4c;4d	2×4e	8f	2×8f	
[2] $C12/c1$ (15)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;+(0,\frac{1}{2},0)$	4c;4d	4a;4b	8f	8f	8f	2×4e	2×8f	
[2] $P12_1/c1$ (14)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2a;2c	4e	4e	2b;2d	4e	4e	2×4e	
[2] $P12_1/c1$ (14)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	4e	2b;2d	2a;2c	4e	4e	4e	2×4e	
Enlarged unit cell, isomorphic										
[2] $P12/c1$	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2a;2c	4g	4g	2b;2d	2×2e	2×2f	2×4g	
[2] $P12/c1$	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	4g	2b;2d	2a;2c	4g	2×2e	2×2f	2×4g	
[3] $P12/c1$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	2a;4g	2b;4g	2c;4g	2d;4g	3×2e	3×2f	3×4g	
[p] $P12/c1$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$ $p=$ prime >2; $u=1,\dots,p-1$	2a;$\frac{p-1}{2}$×4g	2b;$\frac{p-1}{2}$×4g	2c;$\frac{p-1}{2}$×4g	2d;$\frac{p-1}{2}$×4g	p×2e	p×2f	p×4g	
[2] $P12/c1$	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	2a;2d	4g	2b;2c	4g	2e;2f	4g	2×4g	
[2] $P12/c1$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	4g	2b;2c	4g	2a;2d	4g	2e;2f	2×4g	
[2] $P12/n1$	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	2a;2d	4g	2b;2c	4g	4g	2e;2f	2×4g	
[2] $P12/n1$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	4g	2b;2c	4g	2a;2d	2e;2f	4g	2×4g	
[3] $P12/c1$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	2a;4g	2b;4g	2c;4g	2d;4g	2e;4g	2f;4g	3×4g	
[3] $P12/c1$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	2a;4g	2b;4g	2c;4g	2d;4g	2e(f^*);4g	2f(e^*);4g	3×4g	
[3] $P12/c1$	**a**−**c**, **b**, 3**c**	$x,y,\frac{1}{3}(x+z);\ \pm(0,0,\frac{1}{3})$	2a;4g	2b;4g	2c;4g	2d;4g	2e;4g	2f;4g	3×4g	
[3] $P12/c1$	**a**+**c**, **b**, 3**c**	$x,y,\frac{1}{3}(-x+z);\ \pm(0,0,\frac{1}{3})$	2a;4g	2b;4g	2c;4g	2d;4g	2e;4g	2f;4g	3×4g	
[p] $P12/c1$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$ $p=$ prime >2; $u=1,\dots,p-1$	2a;$\frac{p-1}{2}$×4g	2b;$\frac{p-1}{2}$×4g	2c;$\frac{p-1}{2}$×4g	2d;$\frac{p-1}{2}$×4g	2e;$\frac{p-1}{2}$×4g	2f;$\frac{p-1}{2}$×4g	p×4g	
[p] $P12/c1$	**a**+q**c**, **b**, p**c**	$x,y,\frac{1}{p}(-qx+z);+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\dots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$	2a;$\frac{p-1}{2}$×4g	2b;$\frac{p-1}{2}$×4g	2c;$\frac{p-1}{2}$×4g	2d;$\frac{p-1}{2}$×4g	2e;$\frac{p-1}{2}$×4g	2f;$\frac{p-1}{2}$×4g	p×4g	

* cell choice 2 ($P12/n1$)

	Axes	Coordinates		Axes	Coordinates

I Maximal *translationengleiche* subgroups

	Axes	Coordinates		Axes	Coordinates
[2] $P1n1$			$P11a$		
[2] $P121$		$x-\frac{1}{4}, y, z-\frac{1}{4}$	$P121$		$x+\frac{1}{4}, y, z$
[2] $P\bar{1}$			$P\bar{1}$		

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

	Axes	Coordinates		Axes	Coordinates
[2] $A12/n1$	$\mathbf{a}-\mathbf{c}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}(x+z); +(0,\frac{1}{2},0)$	$I12/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z, \frac{1}{2}y, \frac{1}{2}z; +(0,\frac{1}{2},0)$
[2] $A12/n1$	$\mathbf{a}-\mathbf{c}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y, \frac{1}{2}(x+z)+\frac{1}{4}; +(0,\frac{1}{2},0)$	$I12/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z-\frac{1}{4}, \frac{1}{2}y, \frac{1}{2}z-\frac{1}{4}; +(0,\frac{1}{2},0)$
[2] $A12/n1$	$\mathbf{a}-\mathbf{c}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}(x+z); +(0,\frac{1}{2},0)$	$I12/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,\frac{1}{2},0)$
[2] $A12/n1$	$\mathbf{a}-\mathbf{c}, 2\mathbf{b}, 2\mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}(x+z)+\frac{1}{4}; +(0,\frac{1}{2},0)$	$I12/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{a}+2\mathbf{c}$	$x-\frac{1}{2}z-\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z-\frac{1}{4}; +(0,\frac{1}{2},0)$
[2] $P12_1/n1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$P12_1/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$
[2] $P12_1/n1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$	$P12_1/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$

Enlarged unit cell, isomorphic

	Axes	Coordinates		Axes	Coordinates
[2] $P12/n1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$P12/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$
[2] $P12/n1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$	$P12/a1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$
[3] $P12/n1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$	$P12/a1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$
[p] $P12/n1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0,\frac{u}{p},0)$	$P12/a1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0,\frac{u}{p},0)$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$			$p = \text{prime} > 2;\ u = 1,\ldots,p-1$	
[2] $P12/n1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z); +(0,0,\frac{1}{2})$	$P12/a1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $P12/n1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z)+\frac{1}{4}; +(0,0,\frac{1}{2})$	$P12/a1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z-\frac{1}{4}; +(0,0,\frac{1}{2})$
[2] $P12/a1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z); +(0,0,\frac{1}{2})$	$P12/n1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $P12/a1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z)+\frac{1}{4}; +(0,0,\frac{1}{2})$	$P12/n1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z-\frac{1}{4}; +(0,0,\frac{1}{2})$
[3] $P12/n1$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(2x+z); \pm(0,0,\frac{1}{3})$	$P12/a1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$
[3] $P12/n1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$	$P12/a1$	$3\mathbf{a}, \mathbf{b}, \mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-z), y, z; \pm(\frac{1}{3},0,0)$
[3] $P12/n1$	$2\mathbf{a}+\mathbf{c}, \mathbf{b}, \mathbf{a}+2\mathbf{c}$	$\frac{1}{3}(2x-z), y, \frac{1}{3}(-x+2z); \pm(\frac{1}{3},0,\frac{1}{3})$	$P12/a1$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z; \pm(\frac{1}{3},0,0)$
[3] $P12/n1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$P12/a1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$
[p] $P12/n1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$P12/a1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$			$p = \text{prime} > 2;\ u = 1,\ldots,p-1$	
[p] $P12/n1$	$p\mathbf{a}, \mathbf{b}, 2q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-2qz), y, z; +(\frac{u}{p},0,0)$	$P12/a1$	$p\mathbf{a}, \mathbf{b}, q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z; +(\frac{u}{p},0,0)$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$			$p = \text{prime} > 2;\ u = 1,\ldots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

	Axes	Coordinates	2a	2b	2c	2d	2e	2f	4g	
I Maximal *translationengleiche* subgroups										
[2] $P11a$ (7)			$2a$	$2a$	$2a$	$2a$	$2a$	$2a$	$2\times2a$	
[2] $P112$ (3)		$x+\frac{1}{4},y,z$	$2e$	$2e$	$2e$	$2e$	$1a;1b$	$1c;1d$	$2\times2e$	
[2] $P\bar{1}$ (2)			$1a;1d$	$1g;1h$	$1b;1f$	$1c;1e$	$2i$	$2i$	$2\times2i$	
			$1a;1e$	$1f;1g$	$1b;1h$	$1c;1d$	$2i$	$2i$	$2\times2i$	$\Rightarrow$
			$1a;1c$	$1f;1h$	$1b;1g$	$1d;1e$	$2i$	$2i$	$2\times2i$	$\Longrightarrow$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $A112/a$ (15)	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$x,\frac{1}{2}y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$4a;4b$	$4c;4d$	$8f$	$8f$	$2\times4e$	$8f$	$2\times8f$	
[2] $A112/a$ (15)	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;+(0,0,\frac{1}{2})$	$8f$	$8f$	$4c;4d$	$4a;4b$	$8f$	$2\times4e$	$2\times8f$	
[2] $A112/a$ (15)	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$x,\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$8f$	$8f$	$4a;4b$	$4c;4d$	$2\times4e$	$8f$	$2\times8f$	
[2] $A112/a$ (15)	$\mathbf{a},2\mathbf{b},2\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4c;4d$	$4a;4b$	$8f$	$8f$	$8f$	$2\times4e$	$2\times8f$	
[2] $P112_1/a$ (14)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2a;2c$	$4e$	$4e$	$2b;2d$	$4e$	$4e$	$2\times4e$	
[2] $P112_1/a$ (14)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4e$	$2b;2d$	$2a;2c$	$4e$	$4e$	$4e$	$2\times4e$	
Enlarged unit cell, isomorphic										
[2] $P112/a$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2a;2c$	$4g$	$4g$	$2b;2d$	$2\times2e$	$2\times2f$	$2\times4g$	
[2] $P112/a$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4g$	$2b;2d$	$2a;2c$	$4g$	$2\times2e$	$2\times2f$	$2\times4g$	
[3] $P112/a$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4g$	$2b;4g$	$2c;4g$	$2d;4g$	$3\times2e$	$3\times2f$	$3\times4g$	
[p] $P112/a$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4g$	$2b;\frac{p-1}{2}\times4g$	$2c;\frac{p-1}{2}\times4g$	$2d;\frac{p-1}{2}\times4g$	$p\times2e$	$p\times2f$	$p\times4g$	
	$p=$ prime >2; $u=1,\ldots,p-1$									
[2] $P112/a$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;+(0,\frac{1}{2},0)$	$2a;2d$	$4g$	$2b;2c$	$4g$	$2e;2f$	$4g$	$2\times4g$	
[2] $P112/a$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;+(0,\frac{1}{2},0)$	$4g$	$2b;2c$	$4g$	$2a;2d$	$4g$	$2e;2f$	$2\times4g$	
[2] $P112/n$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;+(0,\frac{1}{2},0)$	$2a;2d$	$4g$	$2b;2c$	$4g$	$4g$	$2e;2f$	$2\times4g$	
[2] $P112/n$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;+(0,\frac{1}{2},0)$	$4g$	$2b;2c$	$4g$	$2a;2d$	$2e;2f$	$4g$	$2\times4g$	
[3] $P112/a$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$2a;4g$	$2b;4g$	$2c;4g$	$2d;4g$	$2e;4g$	$2f;4g$	$3\times4g$	
[3] $P112/a$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$2a;4g$	$2b;4g$	$2c;4g$	$2d;4g$	$2e(f^*);4g$	$2f(e^*);4g$	$3\times4g$	
[3] $P112/a$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+y),y,z;\pm(\frac{1}{3},0,0)$	$2a;4g$	$2b;4g$	$2c;4g$	$2d;4g$	$2e;4g$	$2f;4g$	$3\times4g$	
[3] $P112/a$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x-y),y,z;\pm(\frac{1}{3},0,0)$	$2a;4g$	$2b;4g$	$2c;4g$	$2d;4g$	$2e;4g$	$2f;4g$	$3\times4g$	
[p] $P112/a$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$	$2a;\frac{p-1}{2}\times4g$	$2b;\frac{p-1}{2}\times4g$	$2c;\frac{p-1}{2}\times4g$	$2d;\frac{p-1}{2}\times4g$	$2e;\frac{p-1}{2}\times4g$	$2f;\frac{p-1}{2}\times4g$	$p\times4g$	
	$p=$ prime >2; $u=1,\ldots,p-1$									
[p] $P112/a$	$p\mathbf{a},q\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{p}(x-qy),y,z;+(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}\times4g$	$2b;\frac{p-1}{2}\times4g$	$2c;\frac{p-1}{2}\times4g$	$2d;\frac{p-1}{2}\times4g$	$2e;\frac{p-1}{2}\times4g$	$2f;\frac{p-1}{2}\times4g$	$p\times4g$	
	$p=$ prime >2; $u=1,\ldots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$									

[*] cell choice 2 ($P112/n$)

	Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups					
[2] $P11n$			$P11b$		
[2] $P112$		$x-\frac{1}{4}, y-\frac{1}{4}, z$	$P112$		$x, y+\frac{1}{4}, z$
[2] $P\bar{1}$			$P\bar{1}$		
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[2] $B112/n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x+y), y, \frac{1}{2}z, ; +(0,0,\frac{1}{2})$	$I112/b$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $B112/n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, y, \frac{1}{2}z, ; +(0,0,\frac{1}{2})$	$I112/b$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, -\frac{1}{2}x+y-\frac{1}{4}, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $B112/n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x+y), y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$I112/b$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
[2] $B112/n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$I112/b$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, -\frac{1}{2}x+y-\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
[2] $P112_1/n$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$P112_1/b$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $P112_1/n$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$P112_1/b$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
Enlarged unit cell, isomorphic					
[2] $P112/n$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$P112/b$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$
[2] $P112/n$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$P112/b$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$
[3] $P112/n$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$P112/b$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$
[p] $P112/n$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$P112/b$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$
	$p = \text{prime} > 2;\ u = 1,\dots,p-1$			$p = \text{prime} > 2;\ u = 1,\dots,p-1$	
[2] $P112/n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), y, z, ; +(\frac{1}{2},0,0)$	$P112/b$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2},0,0)$
[2] $P112/n$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, y, z; +(\frac{1}{2},0,0)$	$P112/b$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, z; +(\frac{1}{2},0,0)$
[2] $P112/b$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), y, z; +(\frac{1}{2},0,0)$	$P112/n$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z; +(\frac{1}{2},0,0)$
[2] $P112/b$	$2\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4}, y, z; +(\frac{1}{2},0,0)$	$P112/n$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x-\frac{1}{4}, y, z; +(\frac{1}{2},0,0)$
[3] $P112/n$	$3\mathbf{a}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+2y), y, z; \pm(\frac{1}{3},0,0)$	$P112/b$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$
[3] $P112/n$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$	$P112/b$	$\mathbf{a}+\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(-x+y), z; \pm(0,\frac{1}{3},0)$
[3] $P112/n$	$2\mathbf{a}+\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3},\frac{1}{3},0)$	$P112/b$	$\mathbf{a}-\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}(x+y), z; \pm(0,\frac{1}{3},0)$
[3] $P112/n$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$	$P112/b$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$
[p] $P112/n$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p},0,0)$	$P112/b$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p},0,0)$
	$p = \text{prime} > 2;\ u = 1,\dots,p-1$			$p = \text{prime} > 2;\ u = 1,\dots,p-1$	
[p] $P112/n$	$\mathbf{a}+2q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-2qx+y), z; +(0,\frac{u}{p},0)$	$P112/b$	$\mathbf{a}+q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}(-qx+y), z; +(0,\frac{u}{p},0)$
	$p = \text{prime} > 2;\ u = 1,\dots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$			$p = \text{prime} > 2;\ u = 1,\dots,p-1;$ $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

$P2_1/c$ No. 14 $P12_1/c1$ C_{2h}^5

UNIQUE AXIS b, CELL CHOICE 1

Subgroup	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$	$4e$	
I Maximal *translationengleiche* subgroups								
[2] $P1c1$ (7)		$x,y+\frac{1}{4},z$	$2a$	$2a$	$2a$	$2a$	$2\times2a$	
[2] $P12_11$ (4)		$x,y,z+\frac{1}{4}$	$2a$	$2a$	$2a$	$2a$	$2\times2a$	
[2] $P\bar{1}$ (2)			$1a;1g$	$1d;1h$	$1b;1c$	$1e;1f$	$2\times2i$	
			$1a;1h$	$1b;1e$	$1c;1f$	$1d;1g$	$2\times2i$	$\Rightarrow$
			$1a;1e$	$1f;1g$	$1c;1d$	$1b;1h$	$2\times2i$	$\Longrightarrow$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, isomorphic								
[3] $P12_1/c1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$	
[p] $P12_1/c1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d;\frac{p-1}{2}\times4e$	$p\times4e$	
	p = prime > 2; $u = 1,\dots,p-1$							
[2] $P12_1/c1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2a;2b(d^\dagger)$	$4e$	$2c;2d(b^\dagger)$	$4e$	$2\times4e$	
[2] $P12_1/c1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4e$	$2a(c^\dagger);2b$	$4e$	$2c(a^\dagger);2d$	$2\times4e$	
[2] $P12_1/n1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2a;2d(b^\dagger)$	$4e$	$2b(d^\dagger);2c$	$4e$	$2\times4e$	
[2] $P12_1/n1$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4e$	$2a;2d$	$4e$	$2b;2c$	$2\times4e$	
[3] $P12_1/c1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$	
[3] $P12_1/c1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$	
[3] $P12_1/c1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}(x+z);\ \pm(0,0,\frac{1}{3})$	$2a;4e$	$2d;4e$	$2c;4e$	$2b;4e$	$3\times4e$	
[3] $P12_1/c1$	$\mathbf{a}+\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}(-x+z);\ \pm(0,0,\frac{1}{3})$	$2a;4e$	$2d;4e$	$2c;4e$	$2b;4e$	$3\times4e$	
or:	$3\mathbf{a}, \mathbf{b}, -2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+2z),y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$	
[p] $P12_1/c1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d;\frac{p-1}{2}\times4e$	$p\times4e$	
	p = prime > 2; $u = 1,\dots,p-1$							
[p] $P12_1/c1$	$\mathbf{a}+q\mathbf{c}, \mathbf{b}, p\mathbf{c}$	$x,y,\frac{1}{p}(-qx+z);\ +(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4e$	$2b(d^*);\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d(b^*);\frac{p-1}{2}\times4e$	$p\times4e$	
	p = prime > 2; $u = 1,\dots,p-1$; $-\frac{1}{2}(p-1) \le q \le \frac{1}{2}(p-1)$							

† cell choice 3 ($P12_1/a1$)

* $q = 2n+1$; does not apply to cell choice 2 ($P12_1/n1$)

	Axes	Coordinates		Axes	Coordinates

I Maximal *translationengleiche* subgroups

	Axes	Coordinates		Axes	Coordinates
[2] $P1n1$		$x, y+\frac{1}{4}, z$	$P1a1$		$x, y+\frac{1}{4}, z$
[2] $P12_11$		$x-\frac{1}{4}, y, z-\frac{1}{4}$	$P12_11$		$x+\frac{1}{4}, y, z$
[2] $P\bar{1}$			$P\bar{1}$		

II Maximal *klassengleiche* subgroups
Enlarged unit cell, isomorphic

	Axes	Coordinates		Axes	Coordinates
[3] $P12_1/n1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$P12_1/a1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$
[p] $P12_1/n1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$P12_1/a1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$
	p = prime > 2; $u = 1, \ldots, p-1$			p = prime > 2; $u = 1, \ldots, p-1$	
[2] $P12_1/n1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z)$; $+(0, 0, \frac{1}{2})$	$P12_1/a1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0, 0, \frac{1}{2})$
[2] $P12_1/n1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x+\frac{1}{4}, y, \frac{1}{2}(x+z)+\frac{1}{4}$; $+(0, 0, \frac{1}{2})$	$P12_1/a1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z-\frac{1}{4}$; $+(0, 0, \frac{1}{2})$
[2] $P12_1/a1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z)$; $+(0, 0, \frac{1}{2})$	$P12_1/n1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0, 0, \frac{1}{2})$
[2] $P12_1/a1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}(x+z)+\frac{1}{4}$; $+(0, 0, \frac{1}{2})$	$P12_1/n1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x-\frac{1}{4}, y, \frac{1}{2}z-\frac{1}{4}$; $+(0, 0, \frac{1}{2})$
[3] $P12_1/n1$	$\mathbf{a}-2\mathbf{c}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}(2x+z)$; $\pm(0, 0, \frac{1}{3})$	$P12_1/a1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$
[3] $P12_1/n1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$P12_1/a1$	$3\mathbf{a}, \mathbf{b}, -2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+2z), y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $P12_1/n1$	$2\mathbf{a}+\mathbf{c}, \mathbf{b}, \mathbf{a}+2\mathbf{c}$	$\frac{1}{3}(2x-z), y, \frac{1}{3}(-x+2z)$; $\pm(\frac{1}{3}, 0, \frac{1}{3})$	$P12_1/a1$	$3\mathbf{a}, \mathbf{b}, -\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+z), y, z$; $\pm(\frac{1}{3}, 0, 0)$
[3] $P12_1/n1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$P12_1/a1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$
[p] $P12_1/n1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$P12_1/a1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$
	p = prime > 2; $u = 1, \ldots, p-1$		p = prime > 2; $u = 1, \ldots, p-1$		
[p] $P12_1/n1$	$p\mathbf{a}, \mathbf{b}, 2q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-2qz), y, z$; $+(\frac{u}{p}, 0, 0)$	$P12_1/a1$	$p\mathbf{a}, \mathbf{b}, q\mathbf{a}+\mathbf{c}$	$\frac{1}{p}(x-qz), y, z$; $+(\frac{u}{p}, 0, 0)$
	p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$			p = prime > 2; $u = 1, \ldots, p-1$; $-\frac{1}{2}(p-1) \leq q \leq \frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

	Axes	Coordinates	Wyckoff positions				
			$2a$	$2b$	$2c$	$2d$	$4e$
I Maximal *translationengleiche* subgroups							
[2] $P11a$ (7)		$x,y,z+\frac{1}{4}$	$2a$	$2a$	$2a$	$2a$	$2\times2a$
[2] $P112_1$ (4)		$x+\frac{1}{4},y,z$	$2a$	$2a$	$2a$	$2a$	$2\times2a$
[2] $P\bar{1}$ (2)			$1a;1f$	$1c;1h$	$1b;1d$	$1e;1g$	$2\times2i$
			$1a;1h$	$1d;1g$	$1b;1e$	$1c;1f$	$2\times2i$ $\Rightarrow$
			$1a;1g$	$1e;1f$	$1b;1c$	$1d;1h$	$2\times2i$ $\Longrightarrow$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[3] $P112_1/a$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$
[p] $P112_1/a$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d;\frac{p-1}{2}\times4e$	$p\times4e$
	$p=$ prime >2; $u=1,\ldots,p-1$						
[2] $P112_1/a$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$2a;2b(d^\dagger)$	$4e$	$2c;2d(b^\dagger)$	$4e$	$2\times4e$
[2] $P112_1/a$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$4e$	$2a(c^\dagger);2b$	$4e$	$2c(a^\dagger);2d$	$2\times4e$
[2] $P112_1/n$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$2a;2d(b^\dagger)$	$4e$	$2b(d^\dagger);2c$	$4e$	$2\times4e$
[2] $P112_1/n$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$4e$	$2a;2d$	$4e$	$2b;2c$	$2\times4e$
[3] $P112_1/a$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$
[3] $P112_1/a$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$
[3] $P112_1/a$	$3\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+y),y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4e$	$2d;4e$	$2c;4e$	$2b;4e$	$3\times4e$
[3] $P112_1/a$	$3\mathbf{a},\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x-y),y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4e$	$2d;4e$	$2c;4e$	$2b;4e$	$3\times4e$
or:	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}(2x+y),z;\ \pm(0,\frac{1}{3},0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$
[p] $P112_1/a$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d;\frac{p-1}{2}\times4e$	$p\times4e$
	$p=$ prime >2; $u=1,\ldots,p-1$						
[p] $P112_1/a$	$p\mathbf{a},q\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{p}(x-qy),y,z;\ +(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}\times4e$	$2b(d^*);\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d(b^*);\frac{p-1}{2}\times4e$	$p\times4e$
	$p=$ prime >2; $u=1,\ldots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$						

† cell choice 3 ($P112_1/b$)
* $q=2n+1$; does not apply to cell choice 2 ($P112_1/n$)

	Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups					
[2] $P11n$		$x,y,z+\frac{1}{4}$	$P11a$		$x,y,z+\frac{1}{4}$
[2] $P112_1$		$x-\frac{1}{4},y-\frac{1}{4},z$	$P12_11$		$x,y+\frac{1}{4},z$
[2] $P\bar{1}$			$P\bar{1}$		
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, isomorphic					
[3] $P112_1/n$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$P112_1/b$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$
[p] $P112_1/n$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$P112_1/b$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$
	$p=\text{prime}>2;\ u=1,\dots,p-1$			$p=\text{prime}>2;\ u=1,\dots,p-1$	
[2] $P112_1/n$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x+y),y,z;\ +(\frac{1}{2},0,0)$	$P112_1/b$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$
[2] $P112_1/n$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4},y+\frac{1}{4},z;\ +(\frac{1}{2},0,0)$	$P112_1/b$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x-\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$
[2] $P112_1/b$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x+y),y,z;\ +(\frac{1}{2},0,0)$	$P112_1/n$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$
[2] $P112_1/b$	$2\mathbf{a},-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$P112_1/n$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x-\frac{1}{4},y-\frac{1}{4},z;\ +(\frac{1}{2},0,0)$
[3] $P112_1/n$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+2y),y,z;\ \pm(\frac{1}{3},0,0)$	$P112_1/b$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$
[3] $P112_1/n$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$P112_1/b$	$\mathbf{a}-2\mathbf{b},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}(2x+y),z;\ \pm(0,\frac{1}{3},0)$
[3] $P112_1/n$	$2\mathbf{a}+\mathbf{b},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$\frac{1}{3}(2x-y),\frac{1}{3}(-x+2y),z;\ \pm(\frac{1}{3},\frac{1}{3},0)$	$P112_1/b$	$\mathbf{a}-\mathbf{b},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}(x+y),z;\ \pm(0,\frac{1}{3},0)$
[3] $P112_1/n$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$P112_1/b$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$
[p] $P112_1/n$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$P112_1/b$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$
	$p=\text{prime}>2;\ u=1,\dots,p-1$		$p=\text{prime}>2;\ u=1,\dots,p-1$		
[p] $P112_1/n$	$\mathbf{a}+2q\mathbf{b},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}(-2qx+y),z;\ +(0,\frac{u}{p},0)$	$P112_1/b$	$\mathbf{a}+q\mathbf{b},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}(-qx+y),z;\ +(0,\frac{u}{p},0)$
	$p=\text{prime}>2;\ u=1,\dots,p-1;$ $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$			$p=\text{prime}>2;\ u=1,\dots,p-1;$ $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 15, pp. 470–473.

$C2/c$ No. 15 $C12/c1$ C_{2h}^{6}

UNIQUE AXIS b, CELL CHOICE 1

	Axes	Coordinates	Wyckoff positions: $4a$	$4b$	$4c$	$4d$	$4e$	$8f$	
I Maximal *translationengleiche* subgroups									
[2] $C1c1$ (9)			$4a$	$4a$	$4a$	$4a$	$4a$	$2\times4a$	
[2] $C121$ (5)		$x,y,z+\frac{1}{4}$	$4c$	$4c$	$4c$	$4c$	$2a;2b$	$2\times4c$	
[2] $P\bar{1}$ (2)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\mathbf{b},\mathbf{c}$	$2x,x+y,z$	$1a;1b$	$1c;1g$	$1e;1f$	$1d;1h$	$2i$	$2\times2i$	
			$1a;1e$	$1c;1d$	$1g;1h$	$1b;1f$	$2i$	$2\times2i$	$\Rightarrow$
			$1a;1d$	$1b;1f$	$1c;1g$	$1e;1h$	$2i$	$2\times2i$	$\Longrightarrow$
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $P12_1/n1$ (14)			$2a;2b$	$2c;2d$	$4e$	$4e$	$4e$	$2\times4e$	
[2] $P12_1/c1$ (14)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4e$	$4e$	$2a;2d$	$2b;2c$	$4e$	$2\times4e$	
[2] $P12/c1$ (13)			$2a;2b$	$2c;2d$	$4g$	$4g$	$2e;2f$	$2\times4g$	
[2] $P12/n1$ (13)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4g$	$4g$	$2a;2b$	$2c;2d$	$2e;2f$	$2\times4g$	
Enlarged unit cell, isomorphic									
[3] $C12/c1$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$3\times4e$	$3\times8f$	
[p] $C12/c1$	$\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=\text{prime}>2;\ u=1,\ldots,p-1$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8f$	$4c(d^*);$ $\frac{p-1}{2}\times8f$	$4d(c^*);$ $\frac{p-1}{2}\times8f$	$p\times4e$	$p\times8f$	
[3] $C12/c1$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$4e;8f$	$3\times8f$	
[3] $C12/c1$	$3\mathbf{a},\mathbf{b},2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-2z),y,z;\pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$4e;8f$	$3\times8f$	
[3] $C12/c1$	$3\mathbf{a},\mathbf{b},-2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x+2z),y,z;\pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$4e;8f$	$3\times8f$	
[3] $C12/c1$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$4a;8f$	$4b;8f$	$4c;8f$	$4d;8f$	$4e;8f$	$3\times8f$	
[p] $C12/c1$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=\text{prime}>2;\ u=1,\ldots,p-1;$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8f$	$4c;\frac{p-1}{2}\times8f$	$4d;\frac{p-1}{2}\times8f$	$4e;\frac{p-1}{2}\times8f$	$p\times8f$	
[p] $C12/c1$	$p\mathbf{a},\mathbf{b},2q\mathbf{a}+\mathbf{c}$ $p=\text{prime}>2;\ u=1,\ldots,p-1;$ $-\frac{1}{2}(p-1)\leq q\leq\frac{1}{2}(p-1)$	$\frac{1}{p}(x-2qz),y,z;+(\frac{u}{p},0,0)$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8f$	$4c(d^*);$ $\frac{p-1}{2}\times8f$	$4d(c^*);$ $\frac{p-1}{2}\times8f$	$4e;\frac{p-1}{2}\times8f$	$p\times8f$	

$^*\ p=4n-1$

	Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups					
[2] $A1n1$			$I1a1$		
[2] $A121$		$x-\frac{1}{4},y,z-\frac{1}{4}$	$I121$		$x+\frac{1}{4},y,z$
[2] $P\bar{1}$	$\mathbf{a},\mathbf{b},\frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x,y+z,2z$	$P\bar{1}$	$\mathbf{a},\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c}),\mathbf{c}$	$x+y,2y,y+z$
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $P12_1/a1$			$P12_1/c1$		
[2] $P12_1/n1$		$x,y+\frac{1}{4},z+\frac{1}{4}$	$P12_1/a1$		$x-\frac{1}{4},y+\frac{1}{4},z-\frac{1}{4}$
[2] $P12/n1$			$P12/a1$		
[2] $P12/a1$		$x,y+\frac{1}{4},z+\frac{1}{4}$	$P12/c1$		$x-\frac{1}{4},y+\frac{1}{4},z-\frac{1}{4}$
Enlarged unit cell, isomorphic					
[3] $A12/n1$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$I12/a1$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$
[p] $A12/n1$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$I12/a1$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$
	$p=\text{prime}>2;\ u=1,\ldots,p-1$			$p=\text{prime}>2;\ u=1,\ldots,p-1$	
[3] $A12/n1$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}(2x+z);\pm(0,0,\frac{1}{3})$	$I12/a1$	$\mathbf{a},\mathbf{b},2\mathbf{a}+3\mathbf{c}$	$x-\frac{2}{3}z,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$
[3] $A12/n1$	$\mathbf{a}+2\mathbf{c},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}(-2x+z);\ \pm(0,0,\frac{1}{3})$	$I12/a1$	$3\mathbf{a},\mathbf{b},2\mathbf{a}+\mathbf{c}$	$\frac{1}{3}(x-2z),y,z;\ \pm(\frac{1}{3},0,0)$
[3] $A12/n1$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$I12/a1$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$
[3] $A12/n1$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$I12/a1$	$\mathbf{a}-2\mathbf{c},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}(2x+z);\ \pm(0,0,\frac{1}{3})$
[p] $A12/n1$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$	$I12/a1$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$
	$p=\text{prime}>2;\ u=1,\ldots,p-1;$			$p=\text{prime}>2;\ u=1,\ldots,p-1;$	
[p] $A12/n1$	$\mathbf{a}+2q\mathbf{c},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}(-2qx+z);\ +(0,0,\frac{u}{p})$	$I12/a1$	$\mathbf{a}+2q\mathbf{c},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}(-2qx+z);\ +(0,0,\frac{u}{p})$
	$p=\text{prime}>2;\ u=1,\ldots,p-1;$			$p=\text{prime}>2;\ u=1,\ldots,p-1;$	
	$-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$			$-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

	Axes	Coordinates	Wyckoff positions 4a	4b	4c	4d	4e	8f	
I Maximal *translationengleiche* subgroups									
[2] $A11a$ (9)			$4a$	$4a$	$4a$	$4a$	$4a$	$2{\times}4a$	
[2] $A112$ (5)		$x+\frac{1}{4},y,z$	$4c$	$4c$	$4c$	$4c$	$2a;2b$	$2{\times}4c$	
[2] $P\bar{1}$ (2)	$\mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c}), \mathbf{c}$	$x,2y,y+z$	$1a;1d$	$1b;1f$	$1e;1g$	$1c;1h$	$2i$	$2{\times}2i$	
			$1a;1g$	$1b;1c$	$1f;1h$	$1d;1e$	$2i$	$2{\times}2i$	$\Rightarrow$
			$1a;1c$	$1d;1e$	$1b;1f$	$1g;1h$	$2i$	$2{\times}2i$	$\Longrightarrow$
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $P112_1/n$ (14)			$2a;2b$	$2c;2d$	$4e$	$4e$	$4e$	$2{\times}4e$	
[2] $P112_1/a$ (14)		$x,y+\frac{1}{4},z+\frac{1}{4}$	$4e$	$4e$	$2a;2d$	$2b;2c$	$4e$	$2{\times}4e$	
[2] $P112/a$ (13)			$2a;2b$	$2c;2d$	$4g$	$4g$	$2e;2f$	$2{\times}4g$	
[2] $P112/n$ (13)		$x,y+\frac{1}{4},z+\frac{1}{4}$	$4g$	$4g$	$2a;2b$	$2c;2d$	$2e;2f$	$2{\times}4g$	
Enlarged unit cell, isomorphic									
[3] $A112/a$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$3{\times}4e$	$3{\times}8f$	
[p] $A112/a$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime >2; $u=1,\dots,p-1$	$4a;\frac{p-1}{2}{\times}8f$	$4b;\frac{p-1}{2}{\times}8f$	$4c(d^*)$; $\frac{p-1}{2}{\times}8f$	$4d(c^*)$; $\frac{p-1}{2}{\times}8f$	$p{\times}4e$	$p{\times}8f$	
[3] $A112/a$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$4e;8f$	$3{\times}8f$	
[3] $A112/a$	$\mathbf{a}+2\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x,\frac{1}{3}(-2x+y),z;\pm(0,\frac{1}{3},0)$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$4e;8f$	$3{\times}8f$	
[3] $A112/a$	$\mathbf{a}-2\mathbf{b}, 3\mathbf{b}, \mathbf{c}$	$x,\frac{1}{3}(2x+y),z;\pm(0,\frac{1}{3},0)$	$4a;8f$	$4b;8f$	$4d;8f$	$4c;8f$	$4e;8f$	$3{\times}8f$	
[3] $A112/a$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x,y,z,;\pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4c;8f$	$4d;8f$	$4e;8f$	$3{\times}8f$	
[p] $A112/a$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$ p = prime >2; $u=1,\dots,p-1$;	$4a;\frac{p-1}{2}{\times}8f$	$4b;\frac{p-1}{2}{\times}8f$	$4c;\frac{p-1}{2}{\times}8f$	$4d;\frac{p-1}{2}{\times}8f$	$4e;\frac{p-1}{2}{\times}8f$	$p{\times}8f$	
[p] $A112/a$	$\mathbf{a}+2q\mathbf{b}, p\mathbf{b}, \mathbf{c}$	$x,\frac{1}{p}(-2qx+y),z;+(0,\frac{u}{p},0)$ p = prime >2; $u=1,\dots,p-1$; $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$	$4a;\frac{p-1}{2}{\times}8f$	$4b;\frac{p-1}{2}{\times}8f$	$4c(d^*)$; $\frac{p-1}{2}{\times}8f$	$4d(c^*)$; $\frac{p-1}{2}{\times}8f$	$4e;\frac{p-1}{2}{\times}8f$	$p{\times}8f$	

* $p=4n-1$

	Axes	Coordinates		Axes	Coordinates
I Maximal *translationengleiche* subgroups					
[2] $B11n$			$I11b$		
[2] $B112$		$x-\frac{1}{4},y-\frac{1}{4},z$	$I112$		$x,y+\frac{1}{4},z$
[2] $P\bar{1}$	$\frac{1}{2}(\mathbf{a}-\mathbf{c}),\mathbf{b},\mathbf{c}$	$2x,y,x+z$			
			$P\bar{1}$	$\mathbf{a},\mathbf{b},\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$	$x+z,y+z,2z$
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $P112_1/b$			$P112_1/a$		
[2] $P112_1/n$		$x+\frac{1}{4},y,z+\frac{1}{4}$	$P112_1/b$		$x-\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$
[2] $P112/n$			$P112/b$		
[2] $P112/b$		$x+\frac{1}{4},y,z+\frac{1}{4}$	$P112/a$		$x-\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$
Enlarged unit cell, isomorphic					
[3] $B112/n$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$I112/b$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$
[p] $B112/n$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$I112/b$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$
	$p=$ prime $>2;\ u=1,\ldots,p-1$			$p=$ prime $>2;\ u=1,\ldots,p-1$	
[3] $B112/n$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+2y),y,z;\pm(\frac{1}{3},0,0)$	$I112/b$	$3\mathbf{a}+2\mathbf{b},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,-\frac{2}{3}x+y,z;\pm(\frac{1}{3},0,0)$
[3] $B112/n$	$3\mathbf{a},2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x-2y),y,z;\ \pm(\frac{1}{3},0,0)$	$I112/b$	$\mathbf{a}+2\mathbf{b},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}(-2x+y),z;\ \pm(0,\frac{1}{3},0)$
[3] $B112/n$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}z,y,z;\ \pm(\frac{1}{3},0,0)$	$I112/b$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$
[3] $B112/n$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$I112/b$	$3\mathbf{a},-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+2y),y,z;\ \pm(\frac{1}{3},0,0)$
[p] $B112/n$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$	$I112/b$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$
	$p=$ prime $>2;\ u=1,\ldots,p-1;$			$p=$ prime $>2;\ u=1,\ldots,p-1;$	
[p] $B112/n$	$p\mathbf{a},2q\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{p}(x-2qy),y,z;\ +(\frac{u}{p},0,0)$	$I112/b$	$p\mathbf{a},2q\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{p}(x-2qy),y,z;\ +(\frac{u}{p},0,0)$
	$p=$ prime $>2;\ u=1,\ldots,p-1;$ $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$			$p=$ prime $>2;\ u=1,\ldots,p-1;$ $-\frac{1}{2}(p-1)\le q\le\frac{1}{2}(p-1)$	

Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 16, pp. 474–475.

$P222$ No. 16 D_2^1

	Axes	Coordinates	Wyckoff positions											
			$1a$	$1b$	$1c$	$1d$	$1e$	$1f$	$1g$	$1h$	$2i$	$2j$	$2k$	$2l$
						$2m$	$2n$	$2o$	$2p$	$2q$	$2r$	$2s$	$2t$	$4u$
I Maximal *translationengleiche* subgroups														
[2] $P211$ (3)			$1a$	$1a$	$1b$	$1c$	$1b$	$1c$	$1d$	$1d$	$2\times1a$	$2\times1c$	$2\times1b$	$2\times1d$
$\widehat{=}P121$	**c**, **a**, **b**	z,x,y				$2e$	$2e$	$2e$	$2e$	$2e$	$2e$	$2e$	$2e$	$2\times2e$
[2] $P121$ (3)			$1a$	$1c$	$1a$	$1b$	$1c$	$1d$	$1b$	$1d$	$2e$	$2e$	$2e$	$2e$
						$2\times1a$	$2\times1b$	$2\times1c$	$2\times1d$	$2e$	$2e$	$2e$	$2e$	$2\times2e$
[2] $P112$ (3)			$1a$	$1b$	$1c$	$1a$	$1d$	$1b$	$1c$	$1d$	$2e$	$2e$	$2e$	$2e$
						$2e$	$2e$	$2e$	$2e$	$2\times1a$	$2\times1b$	$2\times1c$	$2\times1d$	$2\times2e$
II Maximal *klassengleiche* subgroups														
Enlarged unit cell, non-isomorphic														
[2] $F222$ (22)	2**a**,2**b**,2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$4a;4b$	$8e$	$8f$	$8g$	$8h$	$8i$	$8j$	$4c;4d$	$2\times8e$	$16k$	$16k$	$2\times8j$
(22)						$2\times8f$	$16k$	$16k$	$2\times8i$	$2\times8g$	$16k$	$16k$	$2\times8h$	$2\times16k$
[2] $F222$ (22)	2**a**,2**b**,2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$8e$	$4a;4b$	$8h$	$8i$	$8f$	$8g$	$4c;4d$	$8j$	$2\times8e$	$16k$	$16k$	$2\times8j$
(22)						$16k$	$2\times8i$	$2\times8f$	$16k$	$16k$	$2\times8g$	$2\times8h$	$16k$	$2\times16k$
[2] $F222$ (22)	2**a**,2**b**,2**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$8f$	$8h$	$4a;4b$	$8j$	$8e$	$4c;4d$	$8g$	$8i$	$16k$	$2\times8j$	$2\times8e$	$16k$
(22)						$2\times8f$	$16k$	$16k$	$2\times8i$	$16k$	$2\times8h$	$2\times8g$	$16k$	$2\times16k$
[2] $F222$ (22)	2**a**,2**b**,2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4};\ +(\frac{1}{2},0,0)$	$8g$	$8i$	$8j$	$4a;4b$	$4c;4d$	$8e$	$8f$	$8h$	$16k$	$2\times8e$	$2\times8j$	$16k$
(22)						$16k$	$2\times8f$	$2\times8i$	$16k$	$2\times8g$	$16k$	$16k$	$2\times8h$	$2\times16k$
[2] $A222$ (21)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y,\frac{1}{2}z;\ +(0,\frac{1}{2},0)$	$2a;2b$	$2c;2d$	$4e$	$4g$	$4f$	$4h$	$4k$	$4k$	$4i;4j$	$8l$	$8l$	$2\times4k$
$\widehat{=}C222$	2**b**, 2**c**, **a**	$\frac{1}{2}y,\frac{1}{2}z,x;\ +(\frac{1}{2},0,0)$				$2\times4e$	$8l$	$2\times4f$	$8l$	$2\times4g$	$2\times4h$	$8l$	$8l$	$2\times8l$
[2] $A222$ (21)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(0,\frac{1}{2},0)$	$4e$	$4f$	$2a;2b$	$4k$	$2c;2d$	$4k$	$4g$	$4h$	$8l$	$2\times4k$	$4i;4j$	$8l$
$\widehat{=}C222$	2**b**, 2**c**, **a**	$\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z,x;\ +(\frac{1}{2},0,0)$				$2\times4e$	$8l$	$2\times4f$	$8l$	$8l$	$8l$	$2\times4g$	$2\times4h$	$2\times8l$
[2] $A222$ (21)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4};\ +(0,\frac{1}{2},0)$	$4g$	$4h$	$4k$	$2a;2b$	$4k$	$2c;2d$	$4e$	$4f$	$8l$	$4i;4j$	$2\times4k$	$8l$
$\widehat{=}C222$	2**b**, 2**c**, **a**	$\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4},x;\ +(\frac{1}{2},0,0)$				$8l$	$2\times4e$	$8l$	$2\times4f$	$2\times4g$	$2\times4h$	$8l$	$8l$	$2\times8l$
[2] $A222$ (21)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};+(0,\frac{1}{2},0)$	$4k$	$4k$	$4g$	$4e$	$4h$	$4f$	$2a;2b$	$2c;2d$	$2\times4k$	$8l$	$8l$	$4i;4j$
$\widehat{=}C222$	2**b**, 2**c**, **a**	$\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4},x;+(\frac{1}{2},0,0)$				$8l$	$2\times4e$	$8l$	$2\times4f$	$8l$	$8l$	$2\times4g$	$2\times4h$	$2\times8l$
[2] $B222$ (21)	2**a**, **b**, 2**c**	$\frac{1}{2}x,y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$2a;2b$	$4g$	$2c;2d$	$4e$	$4h$	$4k$	$4f$	$4k$	$2\times4g$	$8l$	$2\times4h$	$8l$
$\widehat{=}C222$	2**c**, 2**a**, **b**	$\frac{1}{2}z,\frac{1}{2}x,y;\ +(0,\frac{1}{2},0)$				$4i;4j$	$8l$	$8l$	$2\times4k$	$2\times4e$	$8l$	$2\times4f$	$8l$	$2\times8l$
[2] $B222$ (21)	2**a**, **b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$4g$	$2a;2b$	$4h$	$4k$	$2c;2d$	$4e$	$4k$	$4f$	$2\times4g$	$8l$	$2\times4h$	$8l$
$\widehat{=}C222$	2**c**, 2**a**, **b**	$\frac{1}{2}z,\frac{1}{2}x+\frac{1}{4},y;\ +(0,\frac{1}{2},0)$				$8l$	$2\times4k$	$4i;4j$	$8l$	$8l$	$2\times4e$	$8l$	$2\times4f$	$2\times8l$
[2] $B222$ (21)	2**a**, **b**, 2**c**	$\frac{1}{2}x,y,\frac{1}{2}z+\frac{1}{4};\ +(\frac{1}{2},0,0)$	$4e$	$4k$	$4f$	$2a;2b$	$4k$	$4g$	$2c;2d$	$4h$	$8l$	$2\times4g$	$8l$	$2\times4h$
$\widehat{=}C222$	2**c**, 2**a**, **b**	$\frac{1}{2}z+\frac{1}{4},\frac{1}{2}x,y;\ +(0,\frac{1}{2},0)$				$8l$	$4i;4j$	$2\times4k$	$8l$	$2\times4e$	$8l$	$2\times4f$	$8l$	$2\times8l$
[2] $B222$ (21)	2**a**, **b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},y,\frac{1}{2}z+\frac{1}{4};+(\frac{1}{2},0,0)$	$4k$	$4e$	$4k$	$4g$	$4f$	$2a;2b$	$4h$	$2c;2d$	$8l$	$2\times4g$	$8l$	$2\times4h$
$\widehat{=}C222$	2**c**, 2**a**, **b**	$\frac{1}{2}z+\frac{1}{4},\frac{1}{2}x+\frac{1}{4},y;+(0,\frac{1}{2},0)$				$2\times4k$	$8l$	$8l$	$4i;4j$	$8l$	$2\times4e$	$8l$	$2\times4f$	$2\times8l$
[2] $C222$ (21)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	$2a;2b$	$4e$	$4g$	$2c;2d$	$4k$	$4f$	$4h$	$4k$	$2\times4e$	$2\times4f$	$8l$	$8l$
						$2\times4g$	$2\times4h$	$8l$	$8l$	$4i;4j$	$8l$	$8l$	$2\times4k$	$2\times8l$
[2] $C222$ (21)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	$4e$	$2a;2b$	$4k$	$4f$	$4g$	$2c;2d$	$4k$	$4h$	$2\times4e$	$2\times4f$	$8l$	$8l$
						$8l$	$8l$	$2\times4g$	$2\times4h$	$8l$	$4i;4j$	$2\times4k$	$8l$	$2\times8l$
[2] $C222$ (21)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;\ +(\frac{1}{2},0,0)$	$4g$	$4k$	$2a;2b$	$4h$	$4e$	$4k$	$2c;2d$	$4f$	$8l$	$8l$	$2\times4e$	$2\times4f$
						$2\times4g$	$2\times4h$	$8l$	$8l$	$8l$	$2\times4k$	$4i;4j$	$8l$	$2\times8l$
[2] $C222$ (21)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$	$4k$	$4g$	$4e$	$4k$	$2a;2b$	$4h$	$4f$	$2c;2d$	$8l$	$8l$	$2\times4e$	$2\times4f$
						$8l$	$8l$	$2\times4g$	$2\times4h$	$2\times4k$	$8l$	$8l$	$4i;4j$	$2\times8l$
[2] $P2_122$ (17)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2a$	$2c$	$2a$	$2b$	$2d$	$2c$	$2b$	$2d$	$4e$	$4e$	$4e$	$4e$
$\widehat{=}P222_1$	**b**, **c**, 2**a**	$y,z,\frac{1}{2}x;\ +(0,0,\frac{1}{2})$				$2\times2a$	$2\times2b$	$4e$	$4e$	$4e$	$2\times2c$	$4e$	$2\times2d$	$2\times4e$
[2] $P2_122$ (17)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$2c$	$2a$	$2d$	$2c$	$2a$	$2b$	$2d$	$2b$	$4e$	$4e$	$4e$	$4e$
$\widehat{=}P222_1$	**b**, **c**, 2**a**	$y,z,\frac{1}{2}x+\frac{1}{4};\ +(0,0,\frac{1}{2})$				$4e$	$4e$	$2\times2a$	$2\times2b$	$2\times2c$	$4e$	$2\times2d$	$4e$	$2\times4e$

	Axes	Coordinates	Wyckoff positions										
			$1a$	$1b$ $2l$	$1c$ $2m$	$1d$ $2n$	$1e$ $2o$	$1f$ $2p$	$1g$ $2q$	$1h$ $2r$	$2i$ $2s$	$2j$ $2t$	$2k$ $4u$
[2] $P22_12$ (17) $\widehat{=}P222_1$	**a**, 2**b**, **c** **c**, **a**, 2**b**	$x,\frac{1}{2}y,z;$ $+(0,\frac{1}{2},0)$ $z,x,\frac{1}{2}y;$ $+(0,0,\frac{1}{2})$	$2a$	$2b$ $2\times2d$	$2c$ $4e$	$2a$ $4e$	$2c$ $4e$	$2b$ $4e$	$2d$ $2\times2a$	$2d$ $2\times2b$	$4e$ $4e$	$4e$ $4e$	$2\times2c$ $2\times4e$
[2] $P22_12$ (17) $\widehat{=}P222_1$	**a**, 2**b**, **c** **c**, **a**, 2**b**	$x,\frac{1}{2}y+\frac{1}{4},z;$ $+(0,\frac{1}{2},0)$ $z,x,\frac{1}{2}y+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	$2c$	$2c$ $4e$	$2a$ $4e$	$2d$ $4e$	$2b$ $4e$	$2d$ $4e$	$2a$ $4e$	$2b$ $4e$	$2\times2c$ $2\times2a$	$2\times2d$ $2\times2b$	$4e$ $2\times4e$
[2] $P222_1$ (17)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$2a$	$2a$ $4e$	$2b$ $4e$	$2c$ $2\times2c$	$2b$ $4e$	$2d$ $2\times2d$	$2c$ $4e$	$2d$ $4e$	$2\times2a$ $4e$	$4e$ $4e$	$2\times2b$ $2\times4e$
[2] $P222_1$ (17)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	$2c$	$2d$ $2\times2b$	$2c$ $2\times2c$	$2a$ $4e$	$2d$ $2\times2d$	$2a$ $4e$	$2b$ $4e$	$2b$ $4e$	$4e$ $4e$	$2\times2a$ $4e$	$4e$ $2\times4e$
Enlarged unit cell, isomorphic													
[2] $P222$	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;$ $+(\frac{1}{2},0,0)$	$1a;1b$	$2i$ $2\times2l$	$1c;1e$ $2m;2o$	$2d;2f$ $2n;2p$	$2k$ $4u$	$2j$ $4u$	$1g;1h$ $2q;2r$	$2l$ $4u$	$2\times2i$ $2s;2t$	$2\times2j$ $4u$	$2\times2k$ $2\times4u$
[2] $P222$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;$ $+(\frac{1}{2},0,0)$	$2i$	$1a;1b$ $2\times2l$	$2k$ $4u$	$2j$ $4u$	$1c;1e$ $2m;2o$	$1d;1f$ $2n;2p$	$2l$ $4u$	$1g;1h$ $2q;2r$	$2\times2i$ $4u$	$2\times2j$ $2s;2t$	$2\times2k$ $2\times4u$
[3] $P222$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;$ $\pm(\frac{1}{3},0,0)$	$1a;2i$	$1b;2i$ $3\times2l$	$1c;2k$ $2m;4u$	$1d;2j$ $2n;4u$	$1e;2k$ $2o;4u$	$1f;2j$ $2p;4u$	$1g;2l$ $2q;4u$	$1h;2l$ $2r;4u$	$3\times2i$ $2s;4u$	$3\times2j$ $2t;4u$	$3\times2k$ $3\times4u$
[p] $P222$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;$ $+(\frac{u}{p},0,0)$ $p=$ prime >2; $u=1,\dots,p-1$	$1a;$ $\frac{p-1}{2}\times2i$	$1b;$ $\frac{p-1}{2}\times2i$ $p\times2l$	$1c;$ $\frac{p-1}{2}\times2k$ $2m;$ $\frac{p-1}{2}\times4u$	$1d;$ $\frac{p-1}{2}\times2j$ $2n;$ $\frac{p-1}{2}\times4u$	$1e;$ $\frac{p-1}{2}\times2k$ $2o;$ $\frac{p-1}{2}\times4u$	$1f;$ $\frac{p-1}{2}\times2j$ $2p;$ $\frac{p-1}{2}\times4u$	$1g;$ $\frac{p-1}{2}\times2l$ $2q;$ $\frac{p-1}{2}\times4u$	$1h;$ $\frac{p-1}{2}\times2l$ $2r;$ $\frac{p-1}{2}\times4u$	$p\times2i$ $2s;$ $\frac{p-1}{2}\times4u$	$p\times2j$ $2t;$ $\frac{p-1}{2}\times4u$	$p\times2k$ $p\times4u$
[2] $P222$	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;$ $+(0,\frac{1}{2},0)$	$1a;1c$	$1b;1e$ $4u$	$2m$ $2\times2m$	$1d;1g$ $2\times2n$	$2o$ $2\times2o$	$1f;1h$ $2\times2p$	$2n$ $2q;2s$	$2p$ $2r;2t$	$2i;2k$ $4u$	$2j;2l$ $4u$	$4u$ $2\times4u$
[2] $P222$	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;$ $+(0,\frac{1}{2},0)$	$2m$	$2o$ $2j;2l$	$1a;1c$ $2\times2m$	$2n$ $2\times2n$	$1b;1e$ $2\times2o$	$2p$ $2\times2p$	$1d;1g$ $4u$	$1f;1h$ $4u$	$4u$ $2q;2s$	$4u$ $2r;2t$	$2i;2k$ $2\times4u$
[3] $P222$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;$ $\pm(0,\frac{1}{3},0)$	$1a;2m$	$1b;2o$ $2l;4u$	$1c;2m$ $3\times2m$	$1d;2n$ $3\times2n$	$1e;2o$ $3\times2o$	$1f;2p$ $3\times2p$	$1g;2n$ $2q;4u$	$1h;2p$ $2r;4u$	$2i;4u$ $2s;4u$	$2j;4u$ $2t;4u$	$2k;4u$ $3\times4u$
[p] $P222$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;$ $+(0,\frac{u}{p},0)$ $p=$ prime >2; $u=1,\dots,p-1$	$1a;$ $\frac{p-1}{2}\times2m$	$1b;$ $\frac{p-1}{2}\times2o$ $2l;$ $\frac{p-1}{2}\times4u$	$1c;$ $\frac{p-1}{2}\times2m$ $p\times2m$	$1d;$ $\frac{p-1}{2}\times2n$ $p\times2n$	$1e;$ $\frac{p-1}{2}\times2o$ $p\times2o$	$1f;$ $\frac{p-1}{2}\times2p$ $p\times2p$	$1g;$ $\frac{p-1}{2}\times2n$ $2q;$ $\frac{p-1}{2}\times4u$	$1h;$ $\frac{p-1}{2}\times2p$ $2r;$ $\frac{p-1}{2}\times4u$	$2i;$ $\frac{p-1}{2}\times4u$ $2s;$ $\frac{p-1}{2}\times4u$	$2j;$ $\frac{p-1}{2}\times4u$ $2t;$ $\frac{p-1}{2}\times4u$	$2k;$ $\frac{p-1}{2}\times4u$ $p\times4u$
[2] $P222$	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$1a;1d$	$1b;1f$ $4u$	$1c;1g$ $2m;2n$	$2q$ $4u$	$1e;1h$ $2o;2p$	$2r$ $4u$	$2s$ $2\times2q$	$2t$ $2\times2r$	$2i;2j$ $2\times2s$	$4u$ $2\times2t$	$2k;2l$ $2\times4u$
[2] $P222$	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	$2q$	$2r$ $2k;2l$	$2s$ $4u$	$1a;1d$ $2m;2n$	$2t$ $4u$	$1b;1f$ $2o;2p$	$1c;1g$ $2\times2q$	$1e;1h$ $2\times2r$	$4u$ $2\times2s$	$2i;2j$ $2\times2t$	$4u$ $2\times4u$
[3] $P222$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$1a;2q$	$1b;2r$ $2l;4u$	$1c;2s$ $2m;4u$	$1d;2q$ $2n;4u$	$1e;2t$ $2o;4u$	$1f;2r$ $2p;4u$	$1g;2s$ $3\times2q$	$1h;2t$ $3\times2r$	$2i;4u$ $3\times2s$	$2j;4u$ $3\times2t$	$2k;4u$ $3\times4u$
[p] $P222$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;$ $+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\dots,p-1$	$1a;$ $\frac{p-1}{2}\times2q$	$1b;$ $\frac{p-1}{2}\times2r$ $2l;$ $\frac{p-1}{2}\times4u$	$1c;$ $\frac{p-1}{2}\times2s$ $2m;$ $\frac{p-1}{2}\times4u$	$1d;$ $\frac{p-1}{2}\times2q$ $2n;$ $\frac{p-1}{2}\times4u$	$1e;$ $\frac{p-1}{2}\times2t$ $2o;$ $\frac{p-1}{2}\times4u$	$1f;$ $\frac{p-1}{2}\times2r$ $2p;$ $\frac{p-1}{2}\times4u$	$1g;$ $\frac{p-1}{2}\times2s$ $p\times2q$	$1h;$ $\frac{p-1}{2}\times2t$ $p\times2r$	$2i;$ $\frac{p-1}{2}\times4u$ $p\times2s$	$2j;$ $\frac{p-1}{2}\times4u$ $p\times2t$	$2k;$ $\frac{p-1}{2}\times4u$ $p\times4u$

$P222_1$ No. 17 D_2^2

	Axes	Coordinates	2a	2b	2c	2d	4e
I Maximal *translationengleiche* subgroups							
[2] $P112_1$ (4)			$2a$	$2a$	$2a$	$2a$	$2\times2a$
[2] $P211$ (3)			$1a$; $1c$	$1b$; $1d$	$2e$	$2e$	$2\times2e$
$\widehat{=}$ $P121$	**c**, **a**, **b**	z,x,y					
[2] $P121$ (3)		$x,y,z+\frac{1}{4}$	$2e$	$2e$	$1a$; $1b$	$1c$; $1d$	$2\times2e$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, non-isomorphic							
[2] $C222_1$ (20)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z;+(\frac{1}{2},0,0)$	$2\times4a$	$8c$	$2\times4b$	$8c$	$2\times8c$
[2] $C222_1$ (20)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;+(\frac{1}{2},0,0)$	$2\times4a$	$8c$	$8c$	$2\times4b$	$2\times8c$
[2] $C222_1$ (20)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$	$8c$	$2\times4a$	$2\times4b$	$8c$	$2\times8c$
[2] $C222_1$ (20)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$	$8c$	$2\times4a$	$8c$	$2\times4b$	$2\times8c$
[2] $P2_122_1$ (18)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z+\frac{1}{4};+(\frac{1}{2},0,0)$	$4c$	$4c$	$2a$; $2b$	$4c$	$2\times4c$
$\widehat{=}$ $P2_12_12$	**c**, 2**a**, **b**	$z+\frac{1}{4},\frac{1}{2}x,y;+(0,\frac{1}{2},0)$					
[2] $P2_122_1$ (18)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z+\frac{1}{4};+(\frac{1}{2},0,0)$	$4c$	$4c$	$4c$	$2a$; $2b$	$2\times4c$
$\widehat{=}$ $P2_12_12$	**c**, 2**a**, **b**	$z+\frac{1}{4},\frac{1}{2}x+\frac{1}{4},y;+(0,\frac{1}{2},0)$					
[2] $P22_12_1$ (18)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;+(0,\frac{1}{2},0)$	$2a$; $2b$	$4c$	$4c$	$4c$	$2\times4c$
$\widehat{=}$ $P2_12_12$	2**b**, **c**, **a**	$\frac{1}{2}y,z,x;+(\frac{1}{2},0,0)$					
[2] $P22_12_1$ (18)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;+(0,\frac{1}{2},0)$	$4c$	$2a$; $2b$	$4c$	$4c$	$2\times4c$
$\widehat{=}$ $P2_12_12$	2**b**, **c**, **a**	$\frac{1}{2}y+\frac{1}{4},z,x;+(\frac{1}{2},0,0)$					
Enlarged unit cell, isomorphic							
[2] $P222_1$	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;+(\frac{1}{2},0,0)$	$2\times2a$	$2\times2b$	$2c$; $2d$	$4e$	$2\times4e$
[2] $P222_1$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;+(\frac{1}{2},0,0)$	$2\times2a$	$2\times2b$	$4e$	$2c$; $2d$	$2\times4e$
[3] $P222_1$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$3\times2a$	$3\times2b$	$2c$; $4e$	$2d$; $4e$	$3\times4e$
[p] $P222_1$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$ $p=$ prime >2; $u=1,\ldots,p-1$	$p\times2a$	$p\times2b$	$2c$; $\frac{p-1}{2}\times4e$	$2d$; $\frac{p-1}{2}\times4e$	$p\times4e$
[2] $P222_1$	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;+(0,\frac{1}{2},0)$	$2a$; $2b$	$4e$	$2\times2c$	$2\times2d$	$2\times4e$
[2] $P222_1$	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;+(0,\frac{1}{2},0)$	$4e$	$2a$; $2b$	$2\times2c$	$2\times2d$	$2\times4e$
[3] $P222_1$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$2a$; $4e$	$2b$; $4e$	$3\times2c$	$3\times2d$	$3\times4e$
[p] $P222_1$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$ $p=$ prime >2; $u=1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times4e$	$2b$; $\frac{p-1}{2}\times4e$	$p\times2c$	$p\times2d$	$p\times4e$
[3] $P222_1$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a$; $4e$	$2b$; $4e$	$2c$; $4e$	$2d$; $4e$	$3\times4e$
[p] $P222_1$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times4e$	$2b$; $\frac{p-1}{2}\times4e$	$2c$; $\frac{p-1}{2}\times4e$	$2d$; $\frac{p-1}{2}\times4e$	$p\times4e$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2_122$	$C\to A$	$\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$	$x\to y\to z\to x$
$P22_12$	$C\to B$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

D_2^3 No. 18 $P2_12_12$

	Axes	Coordinates	Wyckoff positions		
			$2a$	$2b$	$4c$
I Maximal *translationengleiche* subgroups					
[2] $P2_111$ (4)		$x, y+\frac{1}{4}, z$	$2a$	$2a$	$2\times 2a$
$\widehat{=} P12_11$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z, x, y+\frac{1}{4}$			
[2] $P12_11$ (4)		$x+\frac{1}{4}, y, z$	$2a$	$2a$	$2\times 2a$
[2] $P112$ (3)			$1a$; $1d$	$1b$; $1c$	$2\times 2e$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[2] $P2_12_12_1$ (19)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x+\frac{1}{4}, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a$	$4a$	$2\times 4a$
[2] $P2_12_12_1$ (19)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x+\frac{1}{4}, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4a$	$4a$	$2\times 4a$
Enlarged unit cell, isomorphic					
[3] $P2_12_12$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$	$2a$; $4c$	$2b$; $4c$	$3\times 4c$
[p] $P2_12_12$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p},0,0)$	$2a$; $\frac{1}{2}(p-1)\times 4c$	$2b$; $\frac{1}{2}(p-1)\times 4c$	$p\times 4c$
	p = prime > 2; $u = 1, \ldots, p-1$				
[3] $P2_12_12$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$	$2a$; $4c$	$2b$; $4c$	$3\times 4c$
[p] $P2_12_12$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0,\frac{u}{p},0)$	$2a$; $\frac{1}{2}(p-1)\times 4c$	$2b$; $\frac{1}{2}(p-1)\times 4c$	$p\times 4c$
	p = prime > 2; $u = 1, \ldots, p-1$				
[2] $P2_12_12$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2\times 2a$	$2\times 2b$	$2\times 4c$
[2] $P2_12_12$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2\times 2a$	$2\times 2b$	$2\times 4c$
[3] $P2_12_12$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times 2a$	$3\times 2b$	$3\times 4c$
[p] $P2_12_12$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times 2a$	$p\times 2b$	$p\times 4c$
	p = prime; $u = 1, \ldots, p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P22_12_1$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$P2_122_1$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

$P2_12_12_1$ No. 19 D_2^4

	Axes	Coordinates	Wyckoff positions
			$4a$
I Maximal *translationengleiche* subgroups			
[2] $P2_111$ (4)		$x, y+\frac{1}{4}, z$	$2\times 2a$
$\widehat{=}\ P12_11$	**c**, **a**, **b**	$z, x, y+\frac{1}{4}$	
[2] $P12_11$ (4)		$x, y, z+\frac{1}{4}$	$2\times 2a$
[2] $P112_1$ (4)		$x+\frac{1}{4}, y, z$	$2\times 2a$
II Maximal *klassengleiche* subgroups			
Enlarged unit cell, isomorphic			
[3] $P2_12_12_1$	3**a**, **b**, **c**	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 4a$
[p] $P2_12_12_1$	p**a**, **b**, **c**	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$	$p\times 4a$
	p = prime > 2; $u = 0, \ldots, p-1$		
[3] $P2_12_12_1$	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	$3\times 4a$
[p] $P2_12_12_1$	**a**, p**b**, **c**	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$	$p\times 4a$
	p = prime > 2; $u = 0, \ldots, p-1$		
[3] $P2_12_12_1$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	$3\times 4a$
[p] $P2_12_12_1$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z;\ +(0, 0, \frac{u}{p})$	$p\times 4a$
	p = prime > 2; $u = 0, \ldots, p-1$		

D_2^5 No. 20 $C222_1$

	Axes	Coordinates	Wyckoff positions 4a	4b	8c
I Maximal *translationengleiche* subgroups					
[2] $C211$ (5)			$2a$; $2b$	$4c$	$2\times4c$
$\widehat{=} C121$	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$	$-y, x, z$			
[2] $C121$ (5)		$x, y, z+\frac{1}{4}$	$4c$	$2a$; $2b$	$2\times4c$
[2] $P112_1$ (4)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x-y, x+y, z$	$2a$	$2a$	$2\times2a$
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $P2_12_12_1$ (19)		$x+\frac{1}{4}, y, z$	$4a$	$4a$	$2\times4a$
[2] $P22_12_1$ (18)		$x+\frac{1}{4}, y, z$	$2a$; $2b$	$4c$	$2\times4c$
$\widehat{=} P2_12_12$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y, z, x+\frac{1}{4}$			
[2] $P2_122_1$ (18)		$x, y+\frac{1}{4}, z+\frac{1}{4}$	$4c$	$2a$; $2b$	$2\times4c$
$\widehat{=} P2_12_12$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z+\frac{1}{4}, x, y+\frac{1}{4}$			
[2] $P222_1$ (17)			$2a$; $2b$	$2c$; $2d$	$2\times4e$
Enlarged unit cell, isomorphic					
[3] $C222_1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$3\times4a$	$4b$; $8c$	$3\times8c$
[p] $C222_1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$	$p\times4a$	$4b$; $\frac{1}{2}(p-1)\times8c$	$p\times8c$
	p = prime > 2; $u = 1, \ldots, p-1$				
[3] $C222_1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$4a$; $8c$	$3\times4b$	$3\times8c$
[p] $C222_1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$4a$; $\frac{1}{2}(p-1)\times8c$	$p\times4b$	$p\times8c$
	p = prime > 2; $u = 1, \ldots, p-1$				
[3] $C222_1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$4a$; $8c$	$4b$; $8c$	$3\times8c$
[p] $C222_1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$4a$; $\frac{1}{2}(p-1)\times8c$	$4b$; $\frac{1}{2}(p-1)\times8c$	$p\times8c$
	p = prime > 2; $u = 1, \ldots, p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$A2_122$	$C \rightarrow A$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$B22_12$	$C \rightarrow B$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

CONTINUED (*from next page*)

No. 21 $C222$

	Axes	Coordinates	Wyckoff positions 2a	2b	2c	2d	4e	4f	4g	4h	4i	4j	4k	8l
[2] $C222$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0, 0, \frac{1}{2})$	$2a$; $2d$	$2b$; $2c$	$4j$	$4i$	$4e$; $4f$	$8l$	$4g$; $4h$	$8l$	$2\times4i$	$2\times4j$	$2\times4k$	$2\times8l$
[2] $C222$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0, 0, \frac{1}{2})$	$4i$	$4j$	$2b$; $2c$	$2a$; $2d$	$8l$	$4e$; $4f$	$8l$	$4g$; $4h$	$2\times4i$	$2\times4j$	$2\times4k$	$2\times8l$
[3] $C222$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$2a$; $4i$	$2b$; $4j$	$2c$; $4j$	$2d$; $4i$	$4e$; $8l$	$4f$; $8l$	$4g$; $8l$	$4h$; $8l$	$3\times4i$	$3\times4j$	$3\times4k$	$3\times8l$
[p] $C222$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$2a$; $\frac{p-1}{2}\times4i$	$2b$; $\frac{p-1}{2}\times4j$	$2c$; $\frac{p-1}{2}\times4j$	$2d$; $\frac{p-1}{2}\times4i$	$4e$; $\frac{p-1}{2}\times8l$	$4f$; $\frac{p-1}{2}\times8l$	$4g$; $\frac{p-1}{2}\times8l$	$4h$; $\frac{p-1}{2}\times8l$	$p\times4i$	$p\times4j$	$p\times4k$	$p\times8l$
	p = prime > 2;	$u = 1, \ldots, p-1$												

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$A222$	$C \rightarrow A$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$B222$	$C \rightarrow B$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

	Axes	Coordinates	Wyckoff positions									
			$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$4i$ $4k$	$4j$ $8l$
I Maximal *translationengleiche* subgroups												
[2] $C211$ (5) $\widehat{=} C121$	 $-\mathbf{b}, \mathbf{a}, \mathbf{c}$	 $-y, x, z$	$2a$	$2a$	$2b$	$2b$	$2\times2a$	$2\times2b$	$4c$	$4c$	$4c$ $4c$	$4c$ $2\times4c$
[2] $C121$ (5)			$2a$	$2a$	$2b$	$2b$	$4c$	$4c$	$2\times2a$	$2\times2b$	$4c$ $4c$	$4c$ $2\times4c$
[2] $P112$ (3)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\mathbf{c}$	$x-y, x+y, z$	$1a$	$1d$	$1d$	$1a$	$2e$	$2e$	$2e$	$2e$	$2\times1a$ $1b; 1c$	$2\times1d$ $2\times2e$
II Maximal *klassengleiche* subgroups												
Loss of centring translations												
[2] $P2_12_12$ (18)			$2a$	$2b$	$2b$	$2a$	$4c$	$4c$	$4c$	$4c$	$2\times2a$ $4c$	$2\times2b$ $2\times4c$
[2] $P2_122$ (17) $\widehat{=} P222_1$	 $\mathbf{b}, \mathbf{c}, \mathbf{a}$	$x, y+\frac{1}{4}, z$ $y+\frac{1}{4}, z, x$	$2a$	$2a$	$2b$	$2b$	$4e$	$4e$	$2\times2a$	$2\times2b$	$4e$ $2c; 2d$	$4e$ $2\times4e$
[2] $P22_12$ (17) $\widehat{=} P222_1$	 $\mathbf{c}, \mathbf{a}, \mathbf{b}$	$x+\frac{1}{4}, y+\frac{1}{4}, z$ $z, x+\frac{1}{4}, y+\frac{1}{4}$	$2c$	$2c$	$2d$	$2d$	$2\times2c$	$2\times2d$	$4e$	$4e$	$4e$ $2a; 2b$	$4e$ $2\times4e$
[2] $P222$ (16)			$1a; 1e$	$1b; 1c$	$1f; 1g$	$1d; 1h$	$2i; 2k$	$2j; 2l$	$2m; 2o$	$2n; 2p$	$2q; 2t$ $4u$	$2r; 2s$ $2\times4u$
Enlarged unit cell, non-isomorphic												
[2] $I2_12_12_1$ (24)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x+\frac{1}{4}, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4b$	$4b$	$4a$	$4a$	$8d$	$2\times4a$	$2\times4b$	$8d$	$8d$ $2\times4c$	$8d$ $2\times8d$
[2] $I2_12_12_1$ (24)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x+\frac{1}{4}, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4a$	$4a$	$4b$	$4b$	$2\times4a$	$8d$	$8d$	$2\times4b$	$8d$ $2\times4c$	$8d$ $2\times8d$
[2] $I222$ (23)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a; 2c$	$2b; 2d$	$4j$	$4i$	$4e; 4f$	$8k$	$4g; 4h$	$8k$	$2\times4i$ $8k$	$2\times4j$ $2\times8k$
[2] $I222$ (23)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4i$	$4j$	$2b; 2d$	$2a; 2c$	$8k$	$4e; 4f$	$8k$	$4g; 4h$	$2\times4i$ $8k$	$2\times4j$ $2\times8k$
[2] $C222_1$ (20)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a$	$4a$	$4b$	$4b$	$2\times4a$	$8c$	$8c$	$2\times4b$	$8c$ $8c$	$8c$ $2\times8c$
[2] $C222_1$ (20)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4b$	$4b$	$4a$	$4a$	$8c$	$2\times4a$	$2\times4b$	$8c$	$8c$ $8c$	$8c$ $2\times8c$
Enlarged unit cell, isomorphic												
[3] $C222$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3},0,0)$	$2a; 4e$	$2b; 4e$	$2c; 4f$	$2d; 4f$	$3\times4e$	$3\times4f$	$4g; 8l$	$4h; 8l$	$4i; 8l$ $4k; 8l$	$4j; 8l$ $3\times8l$
[p] $C222$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$ p = prime > 2;	$\frac{1}{p}x, y, z; +(\frac{u}{p},0,0)$ $u = 1, \ldots, p-1$	$2a$; $\frac{p-1}{2}\times4e$	$2b$; $\frac{p-1}{2}\times4e$	$2c$; $\frac{p-1}{2}\times4f$	$2d$; $\frac{p-1}{2}\times4f$	$p\times4e$	$p\times4f$	$4g$; $\frac{p-1}{2}\times8l$	$4h$; $\frac{p-1}{2}\times8l$	$4i$; $\frac{p-1}{2}\times8l$ $4k$; $\frac{p-1}{2}\times8l$	$4j$; $\frac{p-1}{2}\times8l$ $p\times8l$
[3] $C222$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0,\frac{1}{3},0)$	$2a; 4g$	$2b; 4g$	$2c; 4h$	$2d; 4h$	$4e; 8l$	$4f; 8l$	$3\times4g$	$3\times4h$	$4i; 8l$ $4k; 8l$	$4j; 8l$ $3\times8l$
[p] $C222$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime > 2;	$x, \frac{1}{p}y, z; +(0,\frac{u}{p},0)$ $u = 1, \ldots, p-1$	$2a$; $\frac{p-1}{2}\times4g$	$2b$; $\frac{p-1}{2}\times4g$	$2c$; $\frac{p-1}{2}\times4h$	$2d$; $\frac{p-1}{2}\times4h$	$4e$; $\frac{p-1}{2}\times8l$	$4f$; $\frac{p-1}{2}\times8l$	$p\times4g$	$p\times4h$	$4i$; $\frac{p-1}{2}\times8l$ $4k$; $\frac{p-1}{2}\times8l$	$4j$; $\frac{p-1}{2}\times8l$ $p\times8l$

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D_2^7 No. 22 $F222$

	Axes	Coordinates	$4a$	$4b$	$4c$	$4d$	$8e$	$8f$	$8g$	$8h$	$8i$	$8j$	$16k$
I Maximal *translationengleiche* subgroups													
[2] $C211$ (5)	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x, y+z, 2z$	$2a$	$2a$	$2b$	$2b$	$2\times 2a$	$4c$	$4c$	$4c$	$4c$	$2\times 2b$	$2\times 4c$
$\widehat{=} C121$	$\mathbf{b}, -\mathbf{a}, \frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$y+z, -x, 2z$											
[2] $C121$ (5)	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$x+z, y, 2z$	$2a$	$2a$	$2b$	$2b$	$4c$	$2\times 2a$	$4c$	$4c$	$2\times 2b$	$4c$	$2\times 4c$
[2] $A112$ (5)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$	$2x, x+y, z$	$2a$	$2a$	$2b$	$2b$	$4c$	$4c$	$2\times 2a$	$2\times 2b$	$4c$	$4c$	$2\times 4c$
II Maximal *klassengleiche* subgroups													
Loss of centring translations													
[2] $A222$ (21)			$2a;2c$	$2b;2d$	$4k$	$4k$	$4i;4j$	$4e;4f$	$4g;4h$	$8l$	$8l$	$2\times 4k$	$2\times 8l$
$\widehat{=} C222$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x											
[2] $A222$ (21)		$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$4k$	$4k$	$2b;2d$	$2a;2c$	$2\times 4k$	$8l$	$8l$	$4g;4h$	$4e;4f$	$4i;4j$	$2\times 8l$
$\widehat{=} C222$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y+\frac{1}{4}, z+\frac{1}{4}, x+\frac{1}{4}$											
[2] $B222$ (21)			$2a;2c$	$2b;2d$	$4k$	$4k$	$4g;4h$	$4i;4j$	$4e;4f$	$8l$	$2\times 4k$	$8l$	$2\times 8l$
$\widehat{=} C222$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y											
[2] $B222$ (21)		$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$4k$	$4k$	$2b;2d$	$2a;2c$	$8l$	$2\times 4k$	$8l$	$4e;4f$	$4i;4j$	$4g;4h$	$2\times 8l$
$\widehat{=} C222$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z+\frac{1}{4}, x+\frac{1}{4}, y+\frac{1}{4}$											
[2] $C222$ (21)			$2a;2c$	$2b;2d$	$4k$	$4k$	$4e;4f$	$4g;4h$	$4i;4j$	$2\times 4k$	$8l$	$8l$	$2\times 8l$
[2] $C222$ (21)		$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$4k$	$4k$	$2b;2d$	$2a;2c$	$8l$	$8l$	$2\times 4k$	$4i;4j$	$4g;4h$	$4e;4f$	$2\times 8l$
[2] $A2_122$ (20)		$x, y+\frac{1}{4}, z$	$4a$	$4a$	$4b$	$4b$	$8c$	$2\times 4a$	$8c$	$2\times 4b$	$8c$	$8c$	$2\times 8c$
$\widehat{=} C222_1$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y+\frac{1}{4}, z, x$											
[2] $A2_122$ (20)		$x+\frac{1}{4}, y, z+\frac{1}{4}$	$4b$	$4b$	$4a$	$4a$	$8c$	$8c$	$2\times 4b$	$8c$	$2\times 4a$	$8c$	$2\times 8c$
$\widehat{=} C222_1$	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y, z+\frac{1}{4}, x+\frac{1}{4}$											
[2] $B22_12$ (20)		$x, y, z+\frac{1}{4}$	$4a$	$4a$	$4b$	$4b$	$8c$	$8c$	$2\times 4a$	$8c$	$8c$	$2\times 4b$	$2\times 8c$
$\widehat{=} C222_1$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z+\frac{1}{4}, x, y$											
[2] $B22_12$ (20)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4b$	$4b$	$4a$	$4a$	$2\times 4b$	$8c$	$8c$	$2\times 4a$	$8c$	$8c$	$2\times 8c$
$\widehat{=} C222_1$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z, x+\frac{1}{4}, y+\frac{1}{4}$											
[2] $C222_1$ (20)		$x+\frac{1}{4}, y, z$	$4a$	$4a$	$4b$	$4b$	$2\times 4a$	$8c$	$8c$	$8c$	$2\times 4b$	$8c$	$2\times 8c$
[2] $C222_1$ (20)		$x, y+\frac{1}{4}, z+\frac{1}{4}$	$4b$	$4b$	$4a$	$4a$	$8c$	$2\times 4b$	$8c$	$8c$	$8c$	$2\times 4a$	$2\times 8c$
Enlarged unit cell, isomorphic													
[3] $F222$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$4a;8e$	$4b;8e$	$4d;8j$	$4c;8j$	$3\times 8e$	$8f;16k$	$8g;16k$	$8h;16k$	$8i;16k$	$3\times 8j$	$3\times 16k$
[p] $F222$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$; p = prime > 2	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$; $u = 1, \ldots, p-1$	$4a$; $\frac{p-1}{2}\times 8e$	$4b$; $\frac{p-1}{2}\times 8e$	$4c(d^*)$; $\frac{p-1}{2}\times 8j$	$4d(c^*)$; $\frac{p-1}{2}\times 8j$	$p\times 8e$	$8f$; $\frac{p-1}{2}\times 16k$	$8g$; $\frac{p-1}{2}\times 16k$	$8h$; $\frac{p-1}{2}\times 16k$	$8i$; $\frac{p-1}{2}\times 16k$	$p\times 8j$	$p\times 16k$
[3] $F222$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$4a;8f$	$4b;8f$	$4d;8i$	$4c;8i$	$8e;16k$	$3\times 8f$	$8g;16k$	$8h;16k$	$3\times 8i$	$8j;16k$	$3\times 16k$
[p] $F222$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$; p = prime > 2	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$; $u = 1, \ldots, p-1$	$4a$; $\frac{p-1}{2}\times 8f$	$4b$; $\frac{p-1}{2}\times 8f$	$4c(d^*)$; $\frac{p-1}{2}\times 8i$	$4d(c^*)$; $\frac{p-1}{2}\times 8i$	$8e$; $\frac{p-1}{2}\times 16k$	$p\times 8f$	$8g$; $\frac{p-1}{2}\times 16k$	$8h$; $\frac{p-1}{2}\times 16k$	$p\times 8i$	$8j$; $\frac{p-1}{2}\times 16k$	$p\times 16k$
[3] $F222$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$4a;8g$	$4b;8g$	$4d;8h$	$4c;8h$	$8e;16k$	$8f;16k$	$3\times 8g$	$3\times 8h$	$8i;16k$	$8j;16k$	$3\times 16k$
[p] $F222$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$; p = prime > 2	$x, y, \frac{1}{p}y; +(0, 0, \frac{u}{p})$; $u = 1, \ldots, p-1$	$4a$; $\frac{p-1}{2}\times 8g$	$4b$; $\frac{p-1}{2}\times 8g$	$4c(d^*)$; $\frac{p-1}{2}\times 8h$	$4d(c^*)$; $\frac{p-1}{2}\times 8h$	$8e$; $\frac{p-1}{2}\times 16k$	$8f$; $\frac{p-1}{2}\times 16k$	$p\times 8g$	$p\times 8h$	$8i$; $\frac{p-1}{2}\times 16k$	$8j$; $\frac{p-1}{2}\times 16k$	$p\times 16k$

${}^*p = 4n-1$

$I222$ No. 23 D_2^8

	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$ $4j$	$4i$ $8k$
I Maximal *translationengleiche* subgroups											
[2] $I211$ (5)			$2a$	$2a$	$2b$	$2b$	$2\times2a$	$2\times2b$	$4c$	$4c$ $4c$	$4c$ $2\times4c$
$\widehat{=}I121$	**c**, **a**, **b**	z,x,y									
$\widehat{=}C121$	−**b**−**c**, **a**, **b**	$-y,x,-y+z$									
[2] $I121$ (5)			$2a$	$2b$	$2b$	$2a$	$4c$	$4c$	$2\times2a$	$2\times2b$ $4c$	$4c$ $2\times4c$
$\widehat{=}C121$	−**a**−**c**, **b**, **a**	$-z,y,x-z$									
[2] $I112$ (5)			$2a$	$2b$	$2a$	$2b$	$4c$	$4c$	$4c$	$4c$ $2\times2b$	$2\times2a$ $2\times4c$
$\widehat{=}A112$	**a**, −**a**+**b**, **c**	$x+y,y,z$									
II Maximal *klassengleiche* subgroups											
Loss of centring translations											
[2] $P22_12_1$ (18)		$x+\frac{1}{4},y,z$	$2a$	$2a$	$2b$	$2b$	$2\times2a$	$2\times2b$	$4c$	$4c$ $4c$	$4c$ $2\times4c$
$\widehat{=}P2_12_12$	**b**, **c**, **a**	$y,z,x+\frac{1}{4}$									
[2] $P2_122_1$ (18)		$x,y+\frac{1}{4},z$	$2a$	$2b$	$2b$	$2a$	$4c$	$4c$	$2\times2a$	$2\times2b$ $4c$	$4c$ $2\times4c$
$\widehat{=}P2_12_12$	**c**, **a**, **b**	$z,x,y+\frac{1}{4}$									
[2] $P2_12_12$ (18)		$x,y,z+\frac{1}{4}$	$2a$	$2b$	$2a$	$2b$	$4c$	$4c$	$4c$	$4c$ $2\times2b$	$2\times2a$ $2\times4c$
[2] $P222$ (16)			$1a;1h$	$1b;1g$	$1d;1e$	$1c;1f$	$2i;2l$	$2j;2k$	$2m;2p$	$2n;2o$ $2r;2s$	$2q;2t$ $2\times4u$
Enlarged unit cell, isomorphic											
[3] $I222$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4e$	$2b;4e$	$2c;4f$	$2d;4f$	$3\times4e$	$3\times4f$	$4g;8k$	$4h;8k$ $4j;8k$	$4i;8k$ $3\times8k$
[p] $I222$	p**a**, **b**, **c** p = prime >2;	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$ $u=1,\dots,p-1$	$2a;$ $\frac{p-1}{2}\times4e$	$2b;$ $\frac{p-1}{2}\times4e$	$2c;$ $\frac{p-1}{2}\times4f$	$2d;$ $\frac{p-1}{2}\times4f$	$p\times4e$	$p\times4f$	$4g;$ $\frac{p-1}{2}\times8k$	$4h;$ $\frac{p-1}{2}\times8k$ $4j;$ $\frac{p-1}{2}\times8k$	$4i;$ $\frac{p-1}{2}\times8k$ $p\times8k$
[3] $I222$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$2a;4g$	$2b;4h$	$2c;4h$	$2d;4g$	$4e;8k$	$4f;8k$	$3\times4g$	$3\times4h$ $4j;8k$	$4i;8k$ $3\times8k$
[p] $I222$	**a**, p**b**, **c** p = prime >2;	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$ $u=1,\dots,p-1$	$2a;$ $\frac{p-1}{2}\times4g$	$2b;$ $\frac{p-1}{2}\times4h$	$2c;$ $\frac{p-1}{2}\times4h$	$2d;$ $\frac{p-1}{2}\times4g$	$4e;$ $\frac{p-1}{2}\times8k$	$4f;$ $\frac{p-1}{2}\times8k$	$p\times4g$	$p\times4h$ $4j;$ $\frac{p-1}{2}\times8k$	$4i;$ $\frac{p-1}{2}\times8k$ $p\times8k$
[3] $I222$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4i$	$2b;4j$	$2c;4i$	$2d;4j$	$4e;8k$	$4f;8k$	$4g;8k$	$4h;8k$ $3\times4j$	$3\times4i$ $3\times8k$
[p] $I222$	**a**, **b**, p**c** p = prime >2;	$x,y,\frac{1}{p}y;\ +(0,0,\frac{u}{p})$ $u=1,\dots,p-1$	$2a;$ $\frac{p-1}{2}\times4i$	$2b;$ $\frac{p-1}{2}\times4j$	$2c;$ $\frac{p-1}{2}\times4i$	$2d;$ $\frac{p-1}{2}\times4j$	$4e;$ $\frac{p-1}{2}\times8k$	$4f;$ $\frac{p-1}{2}\times8k$	$4g;$ $\frac{p-1}{2}\times8k$	$4h;$ $\frac{p-1}{2}\times8k$ $p\times4j$	$p\times4i$ $p\times8k$

D_2^9 No. 24 $I2_12_12_1$

	Axes	Coordinates	4*a*	4*b*	4*c*	8*d*
I Maximal *translationengleiche* subgroups						
[2] $I211$ (5)		$x, y, z+\frac{1}{4}$	$2a; 2b$	$4c$	$4c$	$2\times 4c$
$\widehat{=}\ I121$	**c**, **a**, **b**	$z+\frac{1}{4}, x, y$				
$\widehat{=}\ C121$	$-$**b**$-$**c**, **a**, **c**	$-y, x, -y+z+\frac{1}{4}$				
[2] $I121$ (5)		$x+\frac{1}{4}, y, z$	$4c$	$2a; 2b$	$4c$	$2\times 4c$
$\widehat{=}\ C121$	$-$**a**$-$**c**, **b**, **a**	$-z, y, x-z+\frac{1}{4}$				
[2] $I112$ (5)		$x, y+\frac{1}{4}, z$	$4c$	$4c$	$2a; 2b$	$2\times 4c$
$\widehat{=}\ A112$	**a**, $-$**a**$+$**b**, **c**	$x+y+\frac{1}{4}, y+\frac{1}{4}, z$				
II Maximal *klassengleiche* subgroups						
Loss of centring translations						
[2] $P2_12_12_1$ (19)			$4a$	$4a$	$4a$	$2\times 4a$
[2] $P222_1$ (17)		$x+\frac{1}{4}, y, z+\frac{1}{4}$	$2a; 2b$	$2c; 2d$	$4e$	$2\times 4e$
[2] $P22_12$ (17)		$x, y+\frac{1}{4}, z+\frac{1}{4}$	$2c; 2d$	$4e$	$2a; 2b$	$2\times 4e$
$\widehat{=}\ P222_1$	**c**, **a**, **b**	$z+\frac{1}{4}, x, y+\frac{1}{4}$				
[2] $P2_122$ (17)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4e$	$2a; 2b$	$2c; 2d$	$2\times 4e$
$\widehat{=}\ P222_1$	**b**, **c**, **a**	$y+\frac{1}{4}, z, x+\frac{1}{4}$				
Enlarged unit cell, isomorphic						
[3] $I2_12_12_1$	3**a**, **b**, **c**	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	$3\times 4a$	$4b; 8d$	$4c; 8d$	$3\times 8d$
[p] $I2_12_12_1$	p**a**, **b**, **c**	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$	$p\times 4a$	$4b; \frac{p-1}{2}\times 8d$	$4c; \frac{p-1}{2}\times 8d$	$p\times 8d$
	p = prime > 2; $u = 1, \ldots, p-1$					
[3] $I2_12_12_1$	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	$4a; 8d$	$3\times 4b$	$4c; 8d$	$3\times 8d$
[p] $I2_12_12_1$	**a**, p**b**, **c**	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$	$4a; \frac{p-1}{2}\times 8d$	$p\times 4b$	$4c; \frac{p-1}{2}\times 8d$	$p\times 8d$
	p = prime > 2; $u = 1, \ldots, p-1$					
[3] $I2_12_12_1$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	$4a; 8d$	$4b; 8d$	$3\times 4c$	$3\times 8d$
[p] $I2_12_12_1$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z;\ +(0, 0, \frac{u}{p})$	$4a; \frac{p-1}{2}\times 8d$	$4b; \frac{p-1}{2}\times 8d$	$p\times 4c$	$p\times 8d$
	p = prime > 2; $u = 1, \ldots, p-1$					

*Pmm*2 No. 25 C_{2v}^{1}

	Axes	Coordinates	1*a*	1*b*	1*c*	1*d*	2*e*	2*f*	2*g*	2*h*	4*i*
I Maximal *translationengleiche* subgroups											
[2] *Pm*11 (6)			1*a*	1*a*	1*b*	1*b*	2*c*	2*c*	2×1*a*	2×1*b*	2×2*c*
≙ *P*1*m*1	**c**, **a**, **b**	z,x,y									
[2] *P*1*m*1 (6)			1*a*	1*b*	1*a*	1*b*	2×1*a*	2×1*b*	2*c*	2*c*	2×2*c*
[2] *P*112 (3)			1*a*	1*c*	1*b*	1*d*	2*e*	2*e*	2*e*	2*e*	2×2*e*
II Maximal *klassengleiche* subgroups											
Enlarged unit cell, non-isomorphic											
[2] *Fmm*2 (42)	2**a**,2**b**,2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	2×4*a*	8*c*	8*d*	8*b*	2×8*d*	16*e*	2×8*c*	16*e*	2×16*e*
[2] *Fmm*2 (42)	2**a**,2**b**,2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	8*d*	8*b*	2×4*a*	8*c*	2×8*d*	16*e*	16*e*	2×8*c*	2×16*e*
[2] *Fmm*2 (42)	2**a**,2**b**,2**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	8*c*	2×4*a*	8*b*	8*d*	16*e*	2×8*d*	2×8*c*	16*e*	2×16*e*
[2] *Fmm*2 (42)	2**a**,2**b**,2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	8*b*	8*d*	8*c*	2×4*a*	16*e*	2×8*d*	16*e*	2×8*c*	2×16*e*
[2] *Aem*2 (39)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y,\frac{1}{2}z;\ +(0,\frac{1}{2},0)$	4*a*	4*c*	4*b*	4*c*	8*d*	2×4*c*	8*d*	8*d*	2×8*d*
[2] *Aem*2 (39)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(0,\frac{1}{2},0)$	4*c*	4*a*	4*c*	4*b*	2×4*c*	8*d*	8*d*	8*d*	2×8*d*
[2] *Bme*2 (39)	2**a**, **b**, 2**c**	$\frac{1}{2}x,y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	4*a*	4*b*	4*c*	4*c*	8*d*	8*d*	8*d*	2×4*c*	2×8*d*
≙ *Aem*2	−**b**, 2**a**, 2**c**	$-y,\frac{1}{2}x,\frac{1}{2}z;\ +(0,\frac{1}{2},0)$									
[2] *Bme*2 (39)	2**a**, **b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	4*c*	4*c*	4*a*	4*b*	8*d*	8*d*	2×4*c*	8*d*	2×8*d*
≙ *Aem*2	−**b**, 2**a**, 2**c**	$-y,\frac{1}{2}x+\frac{1}{4},\frac{1}{2}z;\ +(0,\frac{1}{2},0)$									
[2] *Amm*2 (38)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y,\frac{1}{2}z;\ +(0,\frac{1}{2},0)$	2×2*a*	4*d*	2×2*b*	4*e*	2×4*c*	8*f*	2×4*d*	2×4*e*	2×8*f*
[2] *Amm*2 (38)	**a**, 2**b**, 2**c**	$x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(0,\frac{1}{2},0)$	4*d*	2×2*a*	4*e*	2×2*b*	8*f*	2×4*c*	2×4*d*	2×4*e*	2×8*f*
[2] *Bmm*2 (38)	2**a**, **b**, 2**c**	$\frac{1}{2}x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2×2*a*	2×2*b*	4*d*	4*e*	2×4*d*	2×4*e*	2×4*c*	8*f*	2×8*f*
≙ *Amm*2	−**b**, 2**a**, 2**c**	$-y,\frac{1}{2}x,\frac{1}{2}z;\ +(0,\frac{1}{2},0)$									
[2] *Bmm*2 (38)	2**a**, **b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	4*d*	4*e*	2×2*a*	2×4*b*	2×4*d*	2×4*e*	8*f*	2×4*c*	2×8*f*
≙ *Amm*2	−**b**, 2**a**, 2**c**	$-y,\frac{1}{2}x+\frac{1}{4},\frac{1}{2}z;\ +(0,\frac{1}{2},0)$									
[2] *Cmm*2 (35)	2**a**,2**b**,**c**	$\frac{1}{2}x,\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	2*a*; 2*b*	4*e*	4*d*	4*c*	2×4*d*	8*f*	2×4*e*	8*f*	2×8*f*
[2] *Cmm*2 (35)	2**a**,2**b**,**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	4*d*	4*c*	2*a*; 2*b*	4*e*	2×4*d*	8*f*	8*f*	2×4*e*	2×8*f*
[2] *Cmm*2 (35)	2**a**,2**b**,**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;\ +(\frac{1}{2},0,0)$	4*e*	2*a*; 2*b*	4*c*	4*d*	8*f*	2×4*d*	2×4*e*	8*f*	2×8*f*
[2] *Cmm*2 (35)	2**a**,2**b**,**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$	4*c*	4*d*	4*e*	2*a*; 2*b*	8*f*	2×4*d*	8*f*	2×4*e*	2×8*f*
[2] *Pma*2 (28)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	2*a*	2*b*	2*c*	2*c*	4*d*	4*d*	4*d*	2×2*c*	2×4*d*
[2] *Pma*2 (28)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	2*c*	2*c*	2*a*	2*b*	4*d*	4*d*	2×2*c*	4*d*	2×4*d*
[2] *Pbm*2 (28)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2*a*	2*c*	2*b*	2*c*	4*d*	2×2*c*	4*d*	4*d*	2×4*d*
≙ *Pma*2	2**b**, −**a**, **c**	$\frac{1}{2}y,-x,z;\ +(\frac{1}{2},0,0)$									
[2] *Pbm*2 (28)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	2*c*	2*a*	2*c*	2*b*	2×2*c*	4*d*	4*d*	4*d*	2×4*d*
≙ *Pma*2	2**b**, −**a**, **c**	$\frac{1}{2}y+\frac{1}{4},-x,z;\ +(\frac{1}{2},0,0)$									
[2] *Pcc*2 (27)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2*a*	2*b*	2*c*	2*d*	4*e*	4*e*	4*e*	4*e*	2×4*e*
[2] $Pmc2_1$ (26)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2*a*	2*a*	2*b*	2*b*	4*c*	4*c*	2×2*a*	2×2*b*	2×4*c*
[2] $Pcm2_1$ (26)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2*a*	2*b*	2*a*	2*b*	2×2*a*	2×2*b*	4*c*	4*c*	2×4*c*
≙ $Pmc2_1$	**b**, −**a**, 2**c**	$y,-x,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$									

	Axes	Coordinates	$1a$	$1b$	$1c$	$1d$	$2e$	$2f$	$2g$	$2h$	$4i$
Enlarged unit cell, isomorphic											
[2] *Pmm*2	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$1a; 1c$	$1b; 1d$	$2e$	$2f$	$2\times2e$	$2\times2f$	$2g; 2h$	$4i$	$2\times4i$
[2] *Pmm*2	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$2e$	$2f$	$1a; 1c$	$1b; 1d$	$2\times2e$	$2\times2f$	$4i$	$2g; 2h$	$2\times4i$
[3] *Pmm*2	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	$1a; 2e$	$1b; 2f$	$1c; 2e$	$1d; 2f$	$3\times2e$	$3\times2f$	$2g; 4i$	$2h; 4i$	$3\times4i$
[p] *Pmm*2	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$ $p = \text{prime} > 2;\ u = 1, \ldots, p-1$	$1a;$ $\frac{p-1}{2}\times2e$	$1b;$ $\frac{p-1}{2}\times2f$	$1c;$ $\frac{p-1}{2}\times2e$	$1d;$ $\frac{p-1}{2}\times2f$	$p\times2e$	$p\times2f$	$2g;$ $\frac{p-1}{2}\times4i$	$2h;$ $\frac{p-1}{2}\times4i$	$p\times4i$
[2] *Pmm*2	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z;\ +(0, \frac{1}{2}, 0)$	$1a; 1b$	$2g$	$1c; 1d$	$2h$	$2e; 2f$	$4i$	$2\times2g$	$2\times2h$	$2\times4i$
[2] *Pmm*2	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z;\ +(0, \frac{1}{2}, 0)$	$2g$	$1a; 1b$	$2h$	$1c; 1d$	$4i$	$2e; 2f$	$2\times2g$	$2\times2h$	$2\times4i$
[3] *Pmm*2	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	$1a; 2g$	$1b; 2g$	$1c; 2h$	$1d; 2h$	$2e; 4i$	$2f; 4i$	$3\times2g$	$3\times2h$	$3\times4i$
[p] *Pmm*2	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$ $p = \text{prime} > 2;\ u = 1, \ldots, p-1$	$1a;$ $\frac{p-1}{2}\times2g$	$1b;$ $\frac{p-1}{2}\times2g$	$1c;$ $\frac{p-1}{2}\times2h$	$1d;$ $\frac{p-1}{2}\times2h$	$2e;$ $\frac{p-1}{2}\times4i$	$2f;$ $\frac{p-1}{2}\times4i$	$p\times2g$	$p\times2h$	$p\times4i$
[2] *Pmm*2	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0, 0, \frac{1}{2})$	$2\times1a$	$2\times1b$	$2\times1c$	$2\times1d$	$2\times2e$	$2\times2f$	$2\times2g$	$2\times2h$	$2\times4i$
[3] *Pmm*2	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	$3\times1a$	$3\times1b$	$3\times1c$	$3\times1d$	$3\times2e$	$3\times2f$	$3\times2g$	$3\times2h$	$3\times4i$
[p] *Pmm*2	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}y, z;\ +(0, 0, \frac{u}{p})$ $p = \text{prime};\ u = 1, \ldots, p-1$	$p\times1a$	$p\times1b$	$p\times1c$	$p\times1d$	$p\times2e$	$p\times2f$	$p\times2g$	$p\times2h$	$p\times4i$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

*P*2*mm* $A \to B \to C \to A$ $a \to b \to c \to a$ $\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$ $x \to y \to z \to x$

*Pm*2*m* $A \leftarrow B \leftarrow C \leftarrow A$ $a \leftarrow b \leftarrow c \leftarrow a$ $\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$ $x \leftarrow y \leftarrow z \leftarrow x$

$Pmc2_1$ No. 26 C_{2v}^2

	Axes	Coordinates	Wyckoff positions 2a	2b	4c
I Maximal *translationengleiche* subgroups					
[2] $P1c1$ (7)			$2a$	$2a$	$2{\times}2a$
[2] $Pm11$ (6)			$2{\times}1a$	$2{\times}1b$	$2{\times}2c$
$\widehat{=}$ $P1m1$	$\mathbf{c},\mathbf{a},\mathbf{b}$	z,x,y			
[2] $P112_1$ (4)			$2a$	$2a$	$2{\times}2a$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[2] $Cmc2_1$ (36)	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	$2{\times}4a$	$8b$	$2{\times}8b$
[2] $Cmc2_1$ (36)	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	$8b$	$2{\times}4a$	$2{\times}8b$
[2] $Cmc2_1$ (36)	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;\ +(\frac{1}{2},0,0)$	$2{\times}4a$	$8b$	$2{\times}8b$
[2] $Cmc2_1$ (36)	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;\ +(\frac{1}{2},0,0)$	$8b$	$2{\times}4a$	$2{\times}8b$
[2] $Pmn2_1$ (31)	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2{\times}2a$	$4b$	$2{\times}4b$
[2] $Pmn2_1$ (31)	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4b$	$2{\times}2a$	$2{\times}4b$
[2] $Pbc2_1$ (29)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z$	$4a$	$4a$	$2{\times}4a$
$\widehat{=}$ $Pca2_1$	$2\mathbf{b},-\mathbf{a},\mathbf{c}$	$\frac{1}{2}y,-x,z$			
[2] $Pbc2_1$ (29)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z$	$4a$	$4a$	$2{\times}4a$
$\widehat{=}$ $Pca2_1$	$2\mathbf{b},-\mathbf{a},\mathbf{c}$	$\frac{1}{2}y+\frac{1}{4},-x,z$			
Enlarged unit cell, isomorphic					
[2] $Pmc2_1$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2a;\ 2b$	$4c$	$2{\times}4c$
[2] $Pmc2_1$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4c$	$2a;\ 2b$	$2{\times}4c$
[3] $Pmc2_1$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a;\ 4c$	$2b;\ 4c$	$3{\times}4c$
[p] $Pmc2_1$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}{\times}4c$	$2b;\frac{p-1}{2}{\times}4c$	$p{\times}4c$
	p = prime >2; $u=1,\dots,p-1$				
[2] $Pmc2_1$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$2{\times}2a$	$2{\times}2b$	$2{\times}4c$
[2] $Pmc2_1$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$2{\times}2a$	$2{\times}2b$	$2{\times}4c$
[3] $Pmc2_1$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$3{\times}2a$	$3{\times}2b$	$3{\times}4c$
[p] $Pmc2_1$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$p{\times}2a$	$p{\times}2b$	$p{\times}4c$
	p = prime; $u=1,\dots,p-1$				
[3] $Pmc2_1$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3{\times}2a$	$3{\times}2b$	$3{\times}4c$
[p] $Pmc2_1$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}y;\ +(0,0,\frac{u}{p})$	$p{\times}2a$	$p{\times}2b$	$p{\times}4c$
	p = prime >2; $u=1,\dots,p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2_1ma$	$C\rightarrow A$	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
$Pb2_1m$	$B\leftarrow C$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$
$Pcm2_1$		$a\rightleftarrows b$	$\mathbf{a}\rightleftarrows-\mathbf{b}$	$x\rightleftarrows -y$
$P2_1am$	$C\rightarrow A$	$a\rightleftarrows c$	$\mathbf{a}\rightleftarrows-\mathbf{c}$	$x\rightleftarrows -z$
$Pm2_1b$	$B\leftarrow C$	$b\rightleftarrows c$	$\mathbf{b}\rightleftarrows-\mathbf{c}$	$y\rightleftarrows -z$

C_{2v}^3 No. 27 $Pcc2$

	Axes	Coordinates	2a	2b	2c	2d	4e
I Maximal *translationengleiche* subgroups							
[2] $Pc11$ (7)			$2a$	$2a$	$2a$	$2a$	$2\times2a$
$\widehat{=}\ P1c1$	**b**, **a**, −**c**	$y,x,-z$					
[2] $P1c1$ (7)			$2a$	$2a$	$2a$	$2a$	$2\times2a$
[2] $P112$ (3)			$2\times1a$	$2\times1c$	$2\times1b$	$2\times1d$	$2\times2e$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, non-isomorphic							
[2] $Ccc2$ (37)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	$4a;4b$	$8d$	$8d$	$2\times4c$	$2\times8d$
[2] $Ccc2$ (37)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;\ +(\frac{1}{2},0,0)$	$8d$	$2\times4c$	$4a;4b$	$8d$	$2\times8d$
[2] $Ccc2$ (37)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;\ +(\frac{1}{2},0,0)$	$8d$	$4a;4b$	$2\times4c$	$8d$	$2\times8d$
[2] $Ccc2$ (37)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;\ +(\frac{1}{2},0,0)$	$2\times4c$	$8d$	$8d$	$4a;4b$	$2\times8d$
[2] $Pcn2$ (30)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2\times2a$	$2\times2b$	$4c$	$4c$	$2\times4c$
$\widehat{=}\ Pnc2$	**b**, 2**a**, −**c**	$y,\frac{1}{2}x,-z;\ +(0,\frac{1}{2},0)$					
[2] $Pcn2$ (30)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4c$	$4c$	$2\times2a$	$2\times2b$	$2\times4c$
$\widehat{=}\ Pnc2$	**b**, 2**a**, −**c**	$y,\frac{1}{2}x+\frac{1}{4},-z;\ +(0,\frac{1}{2},0)$					
[2] $Pnc2$ (30)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$2\times2a$	$4c$	$2\times2b$	$4c$	$2\times4c$
[2] $Pnc2$ (30)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$4c$	$2\times2a$	$4c$	$2\times2b$	$2\times4c$
Enlarged unit cell, isomorphic							
[2] $Pcc2$	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2a;2c$	$2b;2d$	$4e$	$4e$	$2\times4e$
[2] $Pcc2$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$4e$	$4e$	$2a;2c$	$2b;2d$	$2\times4e$
[3] $Pcc2$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$
[p] $Pcc2$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d;\frac{p-1}{2}\times4e$	$p\times4e$
	p = prime > 2; $u=1,\ldots,p-1$						
[2] $Pcc2$	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$2a;2b$	$4e$	$2c;2d$	$4e$	$2\times4e$
[2] $Pcc2$	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$4e$	$2a;2b$	$4e$	$2c;2d$	$2\times4e$
[3] $Pcc2$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$2a;4e$	$2b;4e$	$2c;4e$	$2d;4e$	$3\times4e$
[p] $Pcc2$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$2c;\frac{p-1}{2}\times4e$	$2d;\frac{p-1}{2}\times4e$	$p\times4e$
	p = prime > 2; $u=1,\ldots,p-1$						
[3] $Pcc2$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times2c$	$3\times2d$	$3\times4e$
[p] $Pcc2$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times2a$	$p\times2b$	$p\times2c$	$p\times2d$	$p\times4e$
	p = prime > 2; $u=1,\ldots,p-1$						

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2aa$	$C\rightarrow A$	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
$Pb2b$	$C\rightarrow B$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

*Pma*2 No. 28 C_{2v}^4

	Axes	Coordinates	Wyckoff positions 2*a*	2*b*	2*c*	4*d*
I Maximal *translationengleiche* subgroups						
[2] $P1a1$ (7)			$2a$	$2a$	$2a$	$2\times 2a$
[2] $Pm11$ (6)		$x+\frac{1}{4}, y, z$	$2c$	$2c$	$1a; 1b$	$2\times 2c$
$\widehat{=}\ P1m1$	**c**, **a**, **b**	$z, x+\frac{1}{4}, y$				
[2] $P112$ (3)			$1a; 1b$	$1c; 1d$	$2e$	$2\times 2e$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $Aea2$ (41)	**a**, 2**b**, 2**c**	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,\frac{1}{2},0)$	$2\times 4a$	$8b$	$8b$	$2\times 8b$
[2] $Aea2$ (41)	**a**, 2**b**, 2**c**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,\frac{1}{2},0)$	$8b$	$2\times 4a$	$8b$	$2\times 8b$
[2] $Ama2$ (40)	**a**, 2**b**, 2**c**	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,\frac{1}{2},0)$	$2\times 4a$	$8c$	$2\times 4b$	$2\times 8c$
[2] $Ama2$ (40)	**a**, 2**b**, 2**c**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,\frac{1}{2},0)$	$8c$	$2\times 4a$	$2\times 4b$	$2\times 8c$
[2] $Pba2$ (32)	**a**, 2**b**, **c**	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$2a; 2b$	$4c$	$4c$	$2\times 4c$
[2] $Pba2$ (32)	**a**, 2**b**, **c**	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$	$4c$	$2a; 2b$	$4c$	$2\times 4c$
[2] $Pmn2_1$ (31)	**a**, **b**, 2**c**	$x+\frac{1}{4}, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4b$	$4b$	$2\times 2a$	$2\times 4b$
[2] $Pcn2$ (30)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2\times 2a$	$2\times 2b$	$4c$	$2\times 4c$
$\widehat{=}\ Pnc2$	**b**, −**a**, 2**c**	$y, -x, \frac{1}{2}z +(0,0,\frac{1}{2})$				
[2] $Pca2_1$ (29)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4a$	$4a$	$4a$	$2\times 4a$
Enlarged unit cell, isomorphic						
[3] $Pma2$	3**a**, **b**, **c**	$\frac{1}{3}x, y, z; \pm(\frac{1}{3},0,0)$	$2a; 4d$	$2b; 4d$	$2c; 4d$	$3\times 4d$
[p] $Pma2$	p**a**, **b**, **c**	$\frac{1}{p}x, y, z; +(\frac{u}{p},0,0)$	$2a; \frac{p-1}{2}\times 4d$	$2b; \frac{p-1}{2}\times 4d$	$2c; \frac{p-1}{2}\times 4d$	$p\times 4d$
		p = prime > 2; $u = 1,\ldots,p-1$				
[2] $Pma2$	**a**, 2**b**, **c**	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$2a; 2b$	$4d$	$2\times 2c$	$2\times 4d$
[2] $Pma2$	**a**, 2**b**, **c**	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$	$4d$	$2a; 2b$	$2\times 2c$	$2\times 4d$
[3] $Pma2$	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z; \pm(0,\frac{1}{3},0)$	$2a; 4d$	$2b; 4d$	$3\times 2c$	$3\times 4d$
[p] $Pma2$	**a**, p**b**, **c**	$x, \frac{1}{p}y, z; +(0,\frac{u}{p},0)$	$2a; \frac{p-1}{2}\times 4d$	$2b; \frac{p-1}{2}\times 4d$	$p\times 2c$	$p\times 4d$
		p = prime > 2; $u = 1,\ldots,p-1$				
[2] $Pma2$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2\times 2a$	$2\times 2b$	$2\times 2c$	$2\times 4d$
[3] $Pma2$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times 2a$	$3\times 2b$	$3\times 2c$	$3\times 4d$
[p] $Pma2$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times 2a$	$p\times 2b$	$p\times 2c$	$p\times 4d$
		p = prime; $u = 1,\ldots,p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2mb$	$A \to B$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Pc2m$	$A \to C$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
$Pbm2$	$A \to B$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
$P2cm$	$A \to C$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
$Pm2a$		$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

C_{2v}^5 No. 29 $Pca2_1$

	Axes	Coordinates	Wyckoff positions
			$4a$
I Maximal *translationengleiche* subgroups			
[2] $Pc11$ (7)		$x+\frac{1}{4}, y, z$	$2\times2a$
$\widehat{=} P1c1$	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$,	$-y, x+\frac{1}{4}, z$	
[2] $P1a1$ (7)			$2\times2a$
[2] $P112_1$ (4)			$2\times2a$
II Maximal *klassengleiche* subgroups			
Enlarged unit cell, non-isomorphic			
[2] $Pna2_1$ (33)	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$	$2\times4a$
[2] $Pna2_1$ (33)	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$	$2\times4a$
Enlarged unit cell, isomorphic			
[3] $Pca2_1$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$3\times4a$
[p] $Pca2_1$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$p\times4a$
		p = prime > 2; $u = 1, \ldots, p-1$	
[2] $Pca2_1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$	$2\times4a$
[2] $Pca2_1$	$\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$	$2\times4a$
[3] $Pca2_1$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$3\times4a$
[p] $Pca2_1$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$p\times4a$
		p = prime; $u = 1, \ldots, p-1$	
[3] $Pca2_1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3\times4a$
[p] $Pca2_1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$p\times4a$
		p = prime > 2; $u = 1, \ldots, p-1$	

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2_1ab$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Pc2_1b$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
$Pbc2_1$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
$P2_1ca$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
$Pb2_1a$	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

$Pnc2$ No. 30 C_{2v}^{6}

	Axes	Coordinates	Wyckoff positions 2*a*	2*b*	4*c*
I Maximal *translationengleiche* subgroups					
[2] $Pn11$ (7) $\widehat{=} P1n1$	**c**, **a**, **b**	z, x, y	$2a$	$2a$	$2 \times 2a$
[2] $P1c1$ (7)		$x, y+\frac{1}{4}, z$	$2a$	$2a$	$2 \times 2a$
[2] $P112$ (3)			$1a$; $1c$	$1b$; $1d$	$2 \times 2e$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[2] $Pnn2$ (34)	2**a**, **b**, **c**	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2a$; $2b$	$4c$	$2 \times 4c$
[2] $Pnn2$ (34)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4}, y, z$; $+(\frac{1}{2}, 0, 0)$	$4c$	$2a$; $2b$	$2 \times 4c$
Enlarged unit cell, isomorphic					
[2] $Pnc2$	2**a**, **b**, **c**	$\frac{1}{2}x, y, z$; $+(\frac{1}{2}, 0, 0)$	$2a$; $2b$	$4c$	$2 \times 4c$
[2] $Pnc2$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4}, y, z$; $+(\frac{1}{2}, 0, 0)$	$4c$	$2a$; $2b$	$2 \times 4c$
[3] $Pnc2$	3**a**, **b**, **c**	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$2a$; $4c$	$2b$; $4c$	$3 \times 4c$
[p] $Pnc2$	p**a**, **b**, **c**	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$ p = prime > 2; $u = 1, \ldots, p-1$	$2a$; $\frac{p-1}{2} \times 4c$	$2b$; $\frac{p-1}{2} \times 4c$	$p \times 4c$
[3] $Pnc2$	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$2a$; $4c$	$2b$; $4c$	$3 \times 4c$
[p] $Pnc2$	**a**, p**b**, **c**	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$ p = prime > 2; $u = 1, \ldots, p-1$	$2a$; $\frac{p-1}{2} \times 4c$	$2b$; $\frac{p-1}{2} \times 4c$	$p \times 4c$
[3] $Pnc2$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$3 \times 2a$	$3 \times 2b$	$3 \times 4c$
[p] $Pnc2$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$ p = prime > 2; $u = 1, \ldots, p-1$	$p \times 2a$	$p \times 2b$	$p \times 4c$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2na$	$c \rightarrow a$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$Pb2n$	$c \rightarrow b$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
$Pcn2$		$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
$P2an$	$c \rightarrow a$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
$Pn2b$	$c \rightarrow b$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

C_{2v}^{7} No. 31 $Pmn2_1$

	Axes	Coordinates	Wyckoff positions $2a$	$4b$
I Maximal *translationengleiche* subgroups				
[2] $P1n1$ (7)			$2a$	$2\times2a$
[2] $Pm11$ (6)			$1a$; $1b$	$2\times2c$
$\widehat{=}P1m1$	**c**, **a**, **b**	z,x,y		
[2] $P112_1$ (4)		$x+\frac{1}{4},y,z$	$2a$	$2\times2a$
II Maximal *klassengleiche* subgroups				
Enlarged unit cell, non-isomorphic				
[2] $Pbn2_1$ (33)	**a**, 2**b**, **c**	$x+\frac{1}{4},\frac{1}{2}y,z$; $+(0,\frac{1}{2},0)$	$4a$	$2\times4a$
$\widehat{=}Pna2_1$	2**b**, **a**, −**c**	$\frac{1}{2}y,x+\frac{1}{4},-z$; $+(\frac{1}{2},0,0)$		
[2] $Pbn2_1$ (33)	**a**, 2**b**, **c**	$x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z$; $+(0,\frac{1}{2},0)$	$4a$	$2\times4a$
$\widehat{=}Pna2_1$	2**b**, **a**, −**c**	$\frac{1}{2}y+\frac{1}{4},x+\frac{1}{4},-z$; $+(\frac{1}{2},0,0)$		
Enlarged unit cell, isomorphic				
[3] $Pmn2_1$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$2a$; $4b$	$3\times4b$
[p] $Pmn2_1$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$	$2a$; $\frac{p-1}{2}\times4b$	$p\times4b$
	p = prime >2; $u=1,\ldots,p-1$			
[2] $Pmn2_1$	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z$; $+(0,\frac{1}{2},0)$	$2\times2a$	$2\times4b$
[2] $Pmn2_1$	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z$; $+(0,\frac{1}{2},0)$	$2\times2a$	$2\times4b$
[3] $Pmn2_1$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$3\times2a$	$3\times4b$
[p] $Pmn2_1$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	$p\times2a$	$p\times4b$
	p = prime; $u=1,\ldots,p-1$			
[3] $Pmn2_1$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times4b$
[p] $Pmn2_1$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times2a$	$p\times4b$
	p = prime >2; $u=1,\ldots,p-1$			

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2_1mn$	$a\rightarrow b\rightarrow c$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
$Pn2_1m$	$c\leftarrow a\leftarrow b$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$
$Pnm2_1$	$a\rightleftarrows b$	$\mathbf{a}\rightleftarrows-\mathbf{b}$	$x\rightleftarrows-y$
$P2_1nm$	$a\rightarrow c$	$\mathbf{a}\rightleftarrows-\mathbf{c}$	$x\rightleftarrows-z$
$Pm2_1n$	$b\rightarrow c$	$\mathbf{b}\rightleftarrows-\mathbf{c}$	$y\rightleftarrows-z$

*Pba*2 No. 32 C_{2v}^8

	Axes	Coordinates	Wyckoff positions 2*a*	2*b*	4*c*
I Maximal *translationengleiche* subgroups					
[2] *Pb*11 (7)		$x+\frac{1}{4},y,z$	2*a*	2*a*	2×2*a*
$\widehat{=}$ *P*1*c*1	**c**, **a**, **b**	$z,x+\frac{1}{4},y$			
[2] *P*1*a*1 (7)		$x,y+\frac{1}{4},z$	2*a*	2*a*	2×2*a*
$\widehat{=}$ *P*1*c*1	**c**, **b**, −**a**	$z,y+\frac{1}{4},-x$			
[2] *P*112 (3)			1*a*; 1*d*	1*b*; 1*c*	2×2*e*
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[2] *Pnn*2 (34)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2×2*a*	2×2*b*	2×4*c*
[2] $Pna2_1$ (33)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	4*a*	4*a*	2×4*a*
[2] $Pbn2_1$ (33)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	4*a*	4*a*	2×4*a*
$\widehat{=}$ $Pna2_1$	**b**, −**a**, 2**c**	$y,-x,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$			
Enlarged unit cell, isomorphic					
[3] *Pba*2	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	2*a*; 4*c*	2*b*; 4*c*	3×4*c*
[*p*] *Pba*2	*p***a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}\times 4c$	$2b;\frac{p-1}{2}\times 4c$	$p\times 4c$
		$p=$ prime >2; $u=1,\ldots,p-1$			
[3] *Pba*2	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	2*a*; 4*c*	2*b*; 4*c*	3×4*c*
[*p*] *Pba*2	**a**, *p***b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$2a;\frac{p-1}{2}\times 4c$	$2b;\frac{p-1}{2}\times 4c$	$p\times 4c$
		$p=$ prime >2; $u=1,\ldots,p-1$			
[2] *Pba*2	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2×2*a*	2×2*b*	2×4*c*
[3] *Pba*2	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	3×2*a*	3×2*b*	3×4*c*
[*p*] *Pba*2	**a**, **b**, *p***c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times 2a$	$p\times 2b$	$p\times 4c$
		$p=$ prime; $u=1,\ldots,p-1$			

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

*P*2*cb*	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
*Pc*2*a*	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

C_{2v}^9 No. 33 $Pna2_1$

	Axes	Coordinates	Wyckoff positions
			$4a$
I Maximal *translationengleiche* subgroups			
[2] $Pn11$ (7)		$x+\frac{1}{4},y,z$	$2\times 2a$
$\widehat{=}\ P1n1$	**c**, **a**, **b**	$z,x+\frac{1}{4},y$	
[2] $P1a1$ (7)		$x,y+\frac{1}{4},z$	$2\times 2a$
$\widehat{=}\ P1c1$	**c**, **b**, −**a**	$z,x+\frac{1}{4},-x$	
[2] $P112_1$ (4)			$2\times 2a$
II Maximal *klassengleiche* subgroups			
Enlarged unit cell, isomorphic			
[3] $Pna2_1$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$3\times 4a$
[p] $Pna2_1$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$p\times 4a$
	$p=$ prime >2; $u=1,\ldots,p-1$		
[3] $Pna2_1$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$3\times 4a$
[p] $Pna2_1$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$p\times 4a$
	$p=$ prime >2; $u=1,\ldots,p-1$		
[3] $Pna2_1$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times 4a$
[p] $Pna2_1$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times 4a$
	$p=$ prime >2; $u=1,\ldots,p-1$		

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2_1nb$	$a\to b;\ c\to a$	$\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$	$x\to y\to z\to x$
$Pc2_1n$	$b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$
$Pbn2_1$	$a\rightleftarrows b$	$\mathbf{a}\rightleftarrows -\mathbf{b}$	$x\rightleftarrows -y$
$P2_1cn$	$a\to c$	$\mathbf{a}\rightleftarrows -\mathbf{c}$	$x\rightleftarrows -z$
$Pn2_1a$	$b\to c$	$\mathbf{b}\rightleftarrows -\mathbf{c}$	$y\rightleftarrows -z$

$Pnn2$ No. 34 C_{2v}^{10}

	Axes	Coordinates	Wyckoff positions		
			$2a$	$2b$	$4c$
I Maximal *translationengleiche* subgroups					
[2] $Pn11$ (7)		$x+\frac{1}{4},y,z$	$2a$	$2a$	$2\times2a$
$\widehat{=}\ P1n1$	**c**, **a**, **b**	$z,x+\frac{1}{4},y$			
$\widehat{=}\ P1c1$	**b**, **a**, −**b**−**c**	$y-z,x+\frac{1}{4},-z$			
[2] $P1n1$ (7)		$x,y+\frac{1}{4},z$	$2a$	$2a$	$2\times2a$
$\widehat{=}\ P1c1$	−**a**, **b**, **a**+**c**	$-x+z,y+\frac{1}{4},z$			
[2] $P112$ (3)			$1a$; $1d$	$1b$;, $1c$	$2\times2e$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[2] $Fdd2$ (43)	2**a**,2**b**,2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$2\times8a$	$16b$	$2\times16b$
[2] $Fdd2$ (43)	2**a**,2**b**,2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$16b$	$2\times8a$	$2\times16b$
[2] $Fdd2$ (43)	2**a**,2**b**,2**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$16b$	$2\times8a$	$2\times16b$
[2] $Fdd2$ (43)	2**a**,2**b**,2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;\ +(\frac{1}{2},0,0)$	$2\times8a$	$16b$	$2\times16b$
Enlarged unit cell, isomorphic					
[3] $Pnn2$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a$; $4c$	$2b$; $4c$	$3\times4c$
[p] $Pnn2$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$2a;\frac{p-1}{2}\times4c$	$2b;\frac{p-1}{2}\times4c$	$p\times4c$
	p = prime > 2 $u=1,\ldots,p-1$				
[3] $Pnn2$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$2a$; $4c$	$2b$; $4c$	$3\times4c$
[p] $Pnn2$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$2a;\frac{p-1}{2}\times4c$	$2b;\frac{p-1}{2}\times4c$	$p\times4c$
	p = prime > 2; $u=1,\ldots,p-1$				
[3] $Pnn2$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times4c$
[p] $Pnn2$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times2a$	$p\times2b$	$p\times4c$
	p = prime > 2; $u=1,\ldots,p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$P2nn$ $c\rightarrow a$ $\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$ $x\rightarrow y\rightarrow z\rightarrow x$

$Pn2n$ $c\rightarrow b$ $\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$ $x\leftarrow y\leftarrow z\leftarrow x$

C_{2v}^{11} No. 35 $Cmm2$

	Axes	Coordinates	$2a$	$2b$	$4c$	$4d$	$4e$	$8f$
I Maximal *translationengleiche* subgroups								
[2] $Cm11$ (8)			$2a$	$2a$	$4b$	$4b$	$2\times2a$	$2\times4b$
$\widehat{=}\ C1m1$	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$	$-y, x, z$						
[2] $C1m1$ (8)			$2a$	$2a$	$4b$	$2\times2a$	$4b$	$2\times4b$
[2] $P112$ (3)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\mathbf{c}$	$x-y, x+y, z$	$1a$	$1d$	$1b; 1c$	$2e$	$2e$	$2\times2e$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $Pba2$ (32)			$2a$	$2b$	$4c$	$4c$	$4c$	$2\times4c$
[2] $Pma2$ (28)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$2c$	$2c$	$2a; 2b$	$4d$	$2\times2c$	$2\times4d$
[2] $Pbm2$ (28)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$2c$	$2c$	$2a; 2b$	$2\times2c$	$4d$	$2\times4d$
$\widehat{=}\ Pma2$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y+\frac{1}{4}, -x-\frac{1}{4}, z$						
[2] $Pmm2$ (25)			$1a; 1d$	$1b; 1c$	$4i$	$2e; 2f$	$2g; 2h$	$2\times4i$
Enlarged unit cell, non-isomorphic								
[2] $Ima2$ (46)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4b$	$4b$	$2\times4a$	$8c$	$2\times4b$	$2\times8c$
[2] $Ibm2$ (46)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4b$	$4b$	$2\times4a$	$2\times4b$	$8c$	$2\times8c$
$\widehat{=}\ Ima2$	$\mathbf{b}, -\mathbf{a}, 2\mathbf{c}$	$y+\frac{1}{4}, -x-\frac{1}{4}, \frac{1}{2}z; +(0,0,\frac{1}{2})$						
[2] $Iba2$ (45)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4b$	$8c$	$8c$	$8c$	$2\times8c$
[2] $Imm2$ (44)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2\times2a$	$2\times2b$	$8e$	$2\times4c$	$2\times4d$	$2\times8e$
[2] $Ccc2$ (37)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4b$	$2\times4c$	$8d$	$8d$	$2\times8d$
[2] $Cmc2_1$ (36)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4a$	$8b$	$8b$	$2\times4a$	$2\times8b$
[2] $Ccm2_1$ (36)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4a$	$8b$	$2\times4a$	$8b$	$2\times8b$
$\widehat{=}\ Cmc2_1$	$\mathbf{b}, -\mathbf{a}, 2\mathbf{c}$	$y, -x, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$						
Enlarged unit cell, isomorphic								
[3] $Cmm2$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3},0,0)$	$2a; 4d$	$2b; 4d$	$4c; 8f$	$3\times4d$	$4e; 8f$	$3\times8f$
[p] $Cmm2$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z;\ +(\frac{u}{p},0,0)$ p = prime > 2; $u = 1, \ldots, p-1$	$2a; \frac{p-1}{2}\times4d$	$2b; \frac{p-1}{2}\times4d$	$4c; \frac{p-1}{2}\times8f$	$p\times4d$	$4e; \frac{p-1}{2}\times8f$	$p\times8f$
[3] $Cmm2$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0,\frac{1}{3},0)$	$2a; 4e$	$2b; 4e$	$4c; 8f$	$4d; 8f$	$3\times4e$	$3\times8f$
[p] $Cmm2$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z;\ +(0,\frac{u}{p},0)$ p = prime > 2; $u = 1, \ldots, p-1$	$2a; \frac{p-1}{2}\times4e$	$2b; \frac{p-1}{2}\times4e$	$4c; \frac{p-1}{2}\times8f$	$4d; \frac{p-1}{2}\times8f$	$p\times4e$	$p\times8f$
[2] $Cmm2$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2\times2a$	$2\times2b$	$2\times4c$	$2\times4d$	$2\times4e$	$2\times8f$
[3] $Cmm2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times4c$	$3\times4d$	$3\times4e$	$3\times8f$
[p] $Cmm2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}y;\ +(0,0,\frac{u}{p})$ p = prime; $u = 1, \ldots, p-1$	$p\times2a$	$p\times2b$	$p\times4c$	$p\times4d$	$p\times4e$	$p\times8f$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$A2mm$	$C \rightarrow A$	$a \rightarrow b \rightarrow c \rightarrow a$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$Bm2m$	$C \rightarrow B$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

$Cmc2_1$ No. 36 C_{2v}^{12}

	Axes	Coordinates	Wyckoff positions 4a	8b
I Maximal *translationengleiche* subgroups				
[2] $C1c1$ (9)			$4a$	$2\times4a$
[2] $Cm11$ (8)			$2\times2a$	$2\times4b$
$\widehat{=}$ $C1m1$	$\mathbf{b},\mathbf{a},-\mathbf{c}$	$y,x,-z$		
[2] $P112_1$ (4)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x-y,x+y,z$	$2a$	$2\times2a$
II Maximal *klassengleiche* subgroups				
Loss of centring translations				
[2] $Pbn2_1$ (33)			$4a$	$2\times4a$
$\widehat{=}$ $Pna2_1$	$\mathbf{b},\mathbf{a},-\mathbf{c}$	$y,x,-z$		
[2] $Pmn2_1$ (31)		$x,y+\frac{1}{4},z$	$2\times2a$	$2\times4b$
[2] $Pbc2_1$ (29)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4a$	$2\times4a$
$\widehat{=}$ $Pca2_1$	$\mathbf{b},\mathbf{a},-\mathbf{c}$	$y+\frac{1}{4},x+\frac{1}{4},-z$		
[2] $Pmc2_1$ (26)			$2a$; $2b$	$2\times4c$
Enlarged unit cell, isomorphic				
[3] $Cmc2_1$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a$; $8b$	$3\times8b$
[p] $Cmc2_1$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$4a$; $\frac{1}{2}(p-1)\times8b$	$p\times8b$
	$p=$ prime >2; $u=1,\ldots,p-1$			
[3] $Cmc2_1$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$3\times4a$	$3\times8b$
[p] $Cmc2_1$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$p\times4a$	$p\times8b$
	$p=$ prime >2; $u=1,\ldots,p-1$			
[3] $Cmc2_1$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times4a$	$3\times8b$
[p] $Cmc2_1$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}y;\ +(0,0,\frac{u}{p})$	$p\times4a$	$p\times8b$
	$p=$ prime >2; $u=1,\ldots,p-1$			

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$A2_1ma$	$C\rightarrow A$	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
$Bb2_1m$	$C\rightarrow B$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$
$Ccm2_1$		$a\rightleftarrows b$	$\mathbf{a}\rightleftarrows-\mathbf{b}$	$x\rightleftarrows -y$
$A2_1am$	$C\rightarrow A$	$a\rightleftarrows c$	$\mathbf{a}\rightleftarrows-\mathbf{c}$	$x\rightleftarrows -z$
$Bm2_1b$	$C\rightarrow B$	$b\rightleftarrows c$	$\mathbf{b}\rightleftarrows-\mathbf{c}$	$y\rightleftarrows -z$

C_{2v}^{13} No. 37 $Ccc2$

Axes	Coordinates		Wyckoff positions			
			$4a$	$4b$	$4c$	$8d$
I Maximal *translationengleiche* subgroups						
[2] $Cc11$ (9)			$4a$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $C1c1$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y, -x, z$				
[2] $C1c1$ (9)			$4a$	$4a$	$4a$	$2\times4a$
[2] $P112$ (3)	$\mathbf{a}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x+y, 2y, z$	$2\times1a$	$2\times1b$	$1c$; $1d$	$2\times2e$
	or: $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x-y, x+y, z$	$2\times1a$	$2\times1d$	$1b$; $1c$	$2\times2e$
II Maximal *klassengleiche* subgroups						
Loss of centring translations						
[2] $Pnn2$ (34)			$2\times2a$	$2\times2b$	$4c$	$2\times4c$
[2] $Pnc2$ (30)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4c$	$4c$	$2a$; $2b$	$2\times4c$
[2] $Pcn2$ (30)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4c$	$4c$	$2a$; $2b$	$2\times4c$
$\widehat{=}$ $Pnc2$	$\mathbf{b}$ $-\mathbf{a}, \mathbf{c}$	$y+\frac{1}{4}, -x-\frac{1}{4}, z$				
[2] $Pcc2$ (27)			$2a$; $2d$	$2b$; $2c$	$4e$	$2\times4e$
Enlarged unit cell, isomorphic						
[3] $Ccc2$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	$4a$; $8d$	$4b$; $8d$	$4c$; $8d$	$3\times8d$
[p] $Ccc2$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z$; $+(\frac{u}{p}, 0, 0)$	$4a$; $\frac{p-1}{2}\times8d$	$4b$; $\frac{p-1}{2}\times8d$	$4c$; $\frac{p-1}{2}\times8d$	$p\times8d$
	p = prime > 2; $u = 1, \ldots, p-1$					
[3] $Ccc2$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	$4a$; $8d$	$4b$; $8d$	$4c$; $8d$	$3\times8d$
[p] $Ccc2$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$	$4a$; $\frac{p-1}{2}\times8d$	$4b$; $\frac{p-1}{2}\times8d$	$4c$; $\frac{p-1}{2}\times8d$	$p\times8d$
	p = prime > 2; $u = 1, \ldots, p-1$					
[3] $Ccc2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$3\times4a$	$3\times4b$	$3\times4c$	$3\times8d$
[p] $Ccc2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$p\times4a$	$p\times4b$	$p\times4c$	$p\times8d$
	p = prime > 2; $u = 1, \ldots, p-1$					

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$A2aa$	$C \rightarrow A$	$c \rightarrow a$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$Bb2b$	$C \rightarrow B$	$c \rightarrow b$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

$Amm2$ No. 38 C_{2v}^{14}

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$4c$	$4d$	$4e$	$8f$
I Maximal *translationengleiche* subgroups								
[2] $A1m1$ (8)			$2a$	$2a$	$2{\times}2a$	$4b$	$4b$	$2{\times}4b$
[2] $Pm11$ (6)	$\mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c}), \frac{1}{2}(\mathbf{b}+\mathbf{c})$	$x, y-z, y+z$	$1a$	$1b$	$2c$	$2{\times}1a$	$2{\times}1b$	$2{\times}2c$
$\widehat{=}\ P1m1$	$\frac{1}{2}(\mathbf{b}+\mathbf{c}), \mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c})$	$y+z, x, y-z$						
[2] $A112$ (5)			$2a$	$2b$	$4c$	$4c$	$4c$	$2{\times}4c$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $Pnm2_1$ (31)			$2a$	$2a$	$2{\times}2a$	$4b$	$4b$	$2{\times}4b$
$\widehat{=}\ Pmn2_1$	$\mathbf{b}, \mathbf{a}, -\mathbf{c}$	$y, -x, z$						
[2] $Pnc2$ (30)			$2a$	$2b$	$4c$	$4c$	$4c$	$2{\times}4c$
[2] $Pmc2_1$ (26)		$x, y+\frac{1}{4}, z$	$2a$	$2b$	$4c$	$2{\times}2a$	$2{\times}2b$	$2{\times}4c$
[2] $Pmm2$ (25)			$1a$; $1b$	$1c$; $1d$	$2e$; $2f$	$2{\times}2g$	$2{\times}2h$	$2{\times}4i$
Enlarged unit cell, non-isomorphic								
[2] $Ima2$ (46)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$4a$	$4b$	$8c$	$8c$	$2{\times}4b$	$2{\times}8c$
[2] $Ima2$ (46)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$4b$	$4a$	$8c$	$2{\times}4b$	$8c$	$2{\times}8c$
[2] $Imm2$ (44)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$2a$; $2b$	$4c$	$2{\times}4c$	$2{\times}4d$	$8e$	$2{\times}8e$
[2] $Imm2$ (44)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$4c$	$2a$; $2b$	$2{\times}4c$	$8e$	$2{\times}4d$	$2{\times}8e$
[2] $Ama2$ (40)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$4a$	$4b$	$8c$	$8c$	$2{\times}4b$	$2{\times}8c$
[2] $Ama2$ (40)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$4b$	$4a$	$8c$	$2{\times}4b$	$8c$	$2{\times}8c$
Enlarged unit cell, isomorphic								
[2] $Amm2$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$2a$; $2b$	$4c$	$2{\times}4c$	$4d$; $4e$	$8f$	$2{\times}8f$
[2] $Amm2$	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$4c$	$2a$; $2b$	$2{\times}4c$	$8f$	$4d$; $4e$	$2{\times}8f$
[3] $Amm2$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	$2a$; $4c$	$2b$; $4c$	$3{\times}4c$	$4d$; $8f$	$4e$; $8f$	$3{\times}8f$
[p] $Amm2$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$	$2a$; $\frac{p-1}{2}{\times}4c$	$2b$; $\frac{p-1}{2}{\times}4c$	$p{\times}4c$	$4d$; $\frac{p-1}{2}{\times}8f$	$4e$; $\frac{p-1}{2}{\times}8f$	$p{\times}8f$
	p = prime > 2; $u = 1, \ldots, p-1$							
[3] $Amm2$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	$2a$; $4d$	$2b$; $4e$	$4c$; $8f$	$3{\times}4d$	$3{\times}4e$	$3{\times}8f$
[p] $Amm2$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$	$2a$; $\frac{p-1}{2}{\times}4d$	$2b$; $\frac{p-1}{2}{\times}4e$	$4c$; $\frac{p-1}{2}{\times}8f$	$p{\times}4d$	$p{\times}4e$	$p{\times}8f$
	p = prime > 2; $u = 1, \ldots, p-1$							
[3] $Amm2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	$3{\times}2a$	$3{\times}2b$	$3{\times}4c$	$3{\times}4d$	$3{\times}4e$	$3{\times}8f$
[p] $Amm2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0, 0, \frac{u}{p})$	$p{\times}2a$	$p{\times}2b$	$p{\times}4c$	$p{\times}4d$	$p{\times}4e$	$p{\times}8f$
	p = prime > 2; $u = 1, \ldots, p-1$							

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$B2mm$	$A \to B$	$a \to b$; $c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Cm2m$	$A \to C$	$a \leftarrow b \leftarrow \mathbf{c}$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

C_{2v}^{15} No. 39 $Aem2$

	Axes	Coordinates	Wyckoff positions 4*a*	4*b*	4*c*	8*d*
I Maximal *translationengleiche* subgroups						
[2] $A1m1$ (8)		$x,y+\frac{1}{4},z$	$4b$	$4b$	$2\times2a$	$2\times4b$
$\widehat{=}\ C1m1$	**c**, −**b**, **a**	$z,-y-\frac{1}{4},x$				
[2] $Pb11$ (7)	**a**, **b**, $\frac{1}{2}$(−**b**+**c**)	$x,y+z,2z$	$2a$	$2a$	$2a$	$2\times2a$
$\widehat{=}\ P1c1$	$\frac{1}{2}$(−**b**+**c**), **a**, **b**	$2z,x,y+z$				
[2] $A112$ (5)			$2\times2a$	$2\times2b$	$4c$	$2\times4c$
II Maximal *klassengleiche* subgroups						
Loss of centring translations						
[2] $Pbc2_1$ (29)		$x,y+\frac{1}{4},z$	$4a$	$4a$	$4a$	$2\times4a$
$\widehat{=}\ Pca2_1$	**b**, −**a**, **c**	$y+\frac{1}{4},-x,z$				
[2] $Pbm2$ (28)			$2\times2a$	$2\times2b$	$2\times2c$	$2\times4d$
$\widehat{=}\ Pma2$	**b**, −**a**, **c**	$y,-x,z$				
[2] $Pcc2$ (27)			$2a;\ 2b$	$2c;\ 2d$	$4e$	$2\times4e$
[2] $Pcm2_1$ (26)		$x,y+\frac{1}{4},z$	$4c$	$4c$	$2a;\ 2b$	$2\times4c$
$\widehat{=}\ Pmc2_1$	**b**, −**a**, **c**	$y+\frac{1}{4},-x,z$				
Enlarged unit cell, non-isomorphic						
[2] $Ibm2$ (46)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2\times4a$	$8c$	$2\times4b$	$2\times8c$
$\widehat{=}\ Ima2$	**b**, 2**a**, −**c**	$y,\frac{1}{2}x,-z;\ +(0,\frac{1}{2},0)$				
[2] $Ibm2$ (46)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$8c$	$2\times4a$	$2\times4b$	$2\times8c$
$\widehat{=}\ Ima2$	**b**, 2**a**, −**c**	$y,\frac{1}{2}x+\frac{1}{4},-z;\ +(0,\frac{1}{2},0)$				
[2] $Iba2$ (45)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$4a;\ 4b$	$8c$	$8c$	$2\times8c$
[2] $Iba2$ (45)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$8c$	$4a;\ 4b$	$8c$	$2\times8c$
[2] $Aea2$ (41)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$2\times4a$	$8b$	$8b$	$2\times8b$
[2] $Aea2$ (41)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$8b$	$2\times4a$	$8b$	$2\times8b$
Enlarged unit cell, isomorphic						
[2] $Aem2$	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	$4a;\ 4b$	$8d$	$2\times4c$	$2\times8d$
[2] $Aem2$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	$8d$	$4a;\ 4b$	$2\times4c$	$2\times8d$
[3] $Aem2$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a;\ 8d$	$4b;\ 8d$	$3\times4c$	$3\times8d$
[p] $Aem2$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$4a;\ \frac{p-1}{2}\times8d$	$4b;\ \frac{p-1}{2}\times8d$	$p\times4c$	$p\times8d$
	p = prime > 2; $u=1,\dots,p-1$					
[3] $Aem2$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;\ 8d$	$4b;\ 8d$	$4c;\ 8d$	$3\times8d$
[p] $Aem2$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$4a;\ \frac{p-1}{2}\times8d$	$4b;\ \frac{p-1}{2}\times8d$	$4c;\ \frac{p-1}{2}\times8d$	$p\times8d$
	p = prime > 2; $u=1,\dots,p-1$					
[3] $Aem2$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times4a$	$3\times4b$	$3\times4c$	$3\times8d$
[p] $Aem2$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times4a$	$p\times4b$	$p\times4c$	$p\times8d$
	p = prime > 2; $u=1,\dots,p-1$					

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$B2em$	$A\rightarrow B;\ C\rightarrow A$	$a\rightarrow b\rightarrow c\rightarrow a$	**a** → **b** → **c** → **a**	$x\rightarrow y\rightarrow z\rightarrow x$
$Cm2e$	$A\rightarrow C;\ C\rightarrow B$	$a\leftarrow b\leftarrow c\leftarrow a$	**a** ← **b** ← **c** ← **a**	$x\leftarrow y\leftarrow z\leftarrow x$
$Bme2$	$A\rightarrow B$	$a\rightleftarrows b$	**a** ⇄ −**b**	$x\rightleftarrows -y$
$C2me$	$A\rightleftarrows C$	$a\rightleftarrows c$	**a** ⇄ −**c**	$x\rightleftarrows -z$
$Ae2m$	$C\rightarrow B$	$b\rightleftarrows c$	**b** ⇄ −**c**	$y\rightleftarrows -z$

$Ama2$ No. 40 C_{2v}^{16}

	Axes	Coordinates	Wyckoff positions 4*a*	4*b*	8*c*
I Maximal *translationengleiche* subgroups					
[2] $A1a1$ (9)			4*a*	4*a*	$4\times 2a$
$\widehat{=}\ C1c1$	$\mathbf{c}, -\mathbf{b}, \mathbf{a}$	$z, -y, x$			
[2] $Pm11$ (6)	$\mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c}), \frac{1}{2}(\mathbf{b}+\mathbf{c})$	$x+\frac{1}{4}, y-z, y+z$	2*c*	1*a*; 1*b*	$2\times 2c$
$\widehat{=}\ P1m1$	$\frac{1}{2}(\mathbf{b}+\mathbf{c}), \mathbf{a}, \frac{1}{2}(\mathbf{b}-\mathbf{c})$	$y+z, x+\frac{1}{4}, y-z$			
[2] $A112$ (5)			2*a*; 2*b*	4*c*	$2\times 4c$
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $Pnn2$ (34)			2*a*; 2*b*	4*c*	$2\times 4c$
[2] $Pna2_1$ (33)		$x, y+\frac{1}{4}, z$	4*a*	4*a*	$2\times 4a$
[2] $Pmn2_1$ (31)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	4*b*	$2\times 2a$	$2\times 4b$
[2] $Pma2$ (28)			2*a*; 2*b*	$2\times 2c$	$2\times 4d$
Enlarged unit cell, isomorphic					
[3] $Ama2$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	4*a*; 8*c*	4*b*; 8*c*	$3\times 8c$
[*p*] $Ama2$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$	4*a*; $\frac{p-1}{2}\times 8c$	4*b*; $\frac{p-1}{2}\times 8c$	$p\times 8c$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$				
[3] $Ama2$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	4*a*; 8*c*	$3\times 4b$	$3\times 8c$
[*p*] $Ama2$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$	4*a*; $\frac{p-1}{2}\times 8c$	$p\times 4b$	$p\times 8c$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$				
[3] $Ama2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	$3\times 4a$	$3\times 4b$	$3\times 8c$
[*p*] $Ama2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}, z;\ +(0, 0, \frac{u}{p})$	$p\times 4a$	$p\times 4b$	$p\times 8c$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$B2mb$	$A \to B;\ C \to A$	$a \to b;\ c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Cc2m$	$A \to C;\ C \to B$	$a \to c;\ c \to b$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
$Bbm2$	$A \to B$	$a \to b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
$C2cm$	$A \rightleftarrows C$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
$Am2a$	$C \to B$	$c \to b$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

C_{2v}^{17} No. 41 $Aea2$

Axes	Coordinates		Wyckoff positions $4a$	$8b$
I Maximal *translationengleiche* subgroups				
[2] $A1n1$ (9)			$4a$	$2\times4a$
$\widehat{=}C1c1$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$z,y+\frac{1}{4},-x$		
[2] $Pb11$ (7)	$\mathbf{a},\mathbf{b},\frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x+\frac{1}{4},y+z,2z$	$2a$	$2\times2a$
$\widehat{=}P1c1$	$\frac{1}{2}(-\mathbf{b}+\mathbf{c}),\mathbf{a},\mathbf{b}$	$2z,x+\frac{1}{4},y+z$		
[2] $A112$ (5)			$2a;2b$	$2\times4c$
II Maximal *klassengleiche* subgroups				
Loss of centring translations				
[2] $Pbn2_1$ (33)		$x,y+\frac{1}{4},z$	$4a$	$2\times4a$
$\widehat{=}Pna2_1$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y+\frac{1}{4},-x,z$		
[2] $Pba2$ (32)			$2a;2b$	$2\times4c$
[2] $Pcn2$ (30)			$2a;2b$	$2\times4c$
$\widehat{=}Pnc2$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y,-x,z$		
[2] $Pca2_1$ (29)		$x,y+\frac{1}{4},z$	$4a$	$2\times4a$
Enlarged unit cell, isomorphic				
[3] $Aea2$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a;8b$	$3\times8b$
[p] $Aea2$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$4a;\frac{p-1}{2}\times8b$	$p\times8b$
	$p=\text{prime}>2;\ u=1,\ldots,p-1$			
[3] $Aea2$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;8b$	$3\times8b$
[p] $Aea2$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$4a;\frac{p-1}{2}\times8b$	$p\times8b$
	$p=\text{prime}>2;\ u=1,\ldots,p-1$			
[3] $Aea2$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times4a$	$3\times8b$
[p] $Aea2$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times4a$	$p\times8b$
	$p=\text{prime}>2;\ u=1,\ldots,p-1$			

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$B2eb$	$A\rightarrow B;\ C\rightarrow A$	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
$Cc2e$	$A\rightarrow C;\ C\rightarrow B$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$
$Bbe2$	$A\rightarrow B$	$a\rightleftarrows b$	$\mathbf{a}\rightleftarrows-\mathbf{b}$	$x\rightleftarrows-y$
$C2ce$	$A\rightleftarrows C$	$a\rightleftarrows c$	$\mathbf{a}\rightleftarrows-\mathbf{c}$	$x\rightleftarrows-z$
$Ae2a$	$C\rightarrow B$	$c\rightleftarrows b$	$\mathbf{b}\rightleftarrows-\mathbf{c}$	$y\rightleftarrows-z$

$Fmm2$ No. 42 C_{2v}^{18}

Axes	Coordinates		Wyckoff positions				
			$4a$	$8b$	$8c$	$8d$	$16e$
I Maximal *translationengleiche* subgroups							
[2] $Cm11$ (8)	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x, y+z, 2z$	$2a$	$4b$	$2\times2a$	$4b$	$2\times4b$
$\widehat{=}C1m1$	$\mathbf{b}, \mathbf{a}, \frac{1}{2}(-\mathbf{b}-\mathbf{c})$	$y-z, x, -2z$					
[2] $C1m1$ (8)	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$x+z, y, 2z$	$2a$	$4b$	$4b$	$2\times2a$	$2\times4b$
[2] $A112$ (5)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$	$2x, x+y, z$	$2a$	$2\times2b$	$4c$	$4c$	$2\times4c$
II Maximal *klassengleiche* subgroups							
Loss of centring translations							
[2] $Aea2$ (41)			$4a$	$8b$	$8b$	$8b$	$2\times8b$
[2] $Bbe2$ (41)			$4a$	$8b$	$8b$	$8b$	$2\times8b$
$\widehat{=}Aea2$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y, -x, z$					
[2] $Ama2$ (40)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4b$	$2\times4a$	$2\times4b$	$8c$	$2\times8c$
[2] $Bbm2$ (40)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4b$	$2\times4a$	$8c$	$2\times4b$	$2\times8c$
$\widehat{=}Ama2$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y+\frac{1}{4}, -x-\frac{1}{4}, z$					
[2] $Aem2$ (39)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4c$	$4a; 4b$	$8d$	$2\times4c$	$2\times8d$
[2] $Bme2$ (39)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4c$	$4a; 4b$	$2\times4c$	$8d$	$2\times8d$
$\widehat{=}Aem2$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y+\frac{1}{4}, -x-\frac{1}{4}, z$					
[2] $Amm2$ (38)			$2a; 2b$	$8f$	$4d; 4e$	$2\times4c$	$2\times8f$
[2] $Bmm2$ (38)			$2a; 2b$	$8f$	$2\times4c$	$4d; 4e$	$2\times8f$
$\widehat{=}Amm2$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y, -x, z$					
[2] $Ccc2$ (37)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4c$	$4a; 4b$	$8d$	$8d$	$2\times8d$
[2] $Cmc2_1$ (36)		$x, y+\frac{1}{4}, z$	$4a$	$8b$	$2\times4a$	$8b$	$2\times8b$
[2] $Ccm2_1$ (36)		$x+\frac{1}{4}, y, z$	$4a$	$8b$	$8b$	$2\times4a$	$2\times8b$
$\widehat{=}Cmc2_1$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y, -x-\frac{1}{4}, z$					
[2] $Cmm2$ (35)			$2a; 2b$	$2\times4c$	$2\times4e$	$2\times4d$	$2\times8f$
Enlarged unit cell, isomorphic							
[3] $Fmm2$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$4a; 8d$	$8b; 16e$	$8c; 16e$	$3\times8d$	$3\times16e$
[p] $Fmm2$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$4a; \frac{p-1}{2}\times8d$	$8b; \frac{p-1}{2}\times16e$	$8c; \frac{p-1}{2}\times16e$	$p\times8d$	$p\times16e$
	p = prime > 2; $u = 1, \ldots, p-1$						
[3] $Fmm2$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$4a; 8c$	$8b; 16e$	$3\times8c$	$8d; 16e$	$3\times16e$
[p] $Fmm2$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$4a; \frac{p-1}{2}\times8c$	$8b; \frac{p-1}{2}\times16e$	$p\times8c$	$8d; \frac{p-1}{2}\times16e$	$p\times16e$
	p = prime > 2; $u = 1, \ldots, p-1$						
[3] $Fmm2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3\times4a$	$3\times8b$	$3\times8c$	$3\times8d$	$3\times16e$
[p] $Fmm2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$p\times4a$	$p\times8b$	$p\times8c$	$p\times8d$	$p\times16e$
	p = prime > 2; $u = 1, \ldots, p-1$						

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$F2mm$	$A \to B \to C \to A$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Fm2m$	$A \leftarrow B \leftarrow C \leftarrow A$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

C_{2v}^{19} No. 43 $Fdd2$

	Axes	Coordinates	Wyckoff positions 8*a*	16*b*
I Maximal *translationengleiche* subgroups				
[2] $Cc11$ (9)	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$x+\frac{1}{8}, y+z, 2z$	$4a$	$2\times4a$
$\widehat{=}$ $C1c1$	$\mathbf{b}, -\mathbf{a}, \frac{1}{2}(-\mathbf{b}+\mathbf{c})$	$y+z, -x-\frac{1}{8}, 2z$		
[2] $C1c1$ (9)	$\mathbf{a}, \mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$x+z, y+\frac{1}{8}, 2z$	$4a$	$2\times4a$
[2] $A112$ (5)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$	$2x, x+y, z$	$2a; 2b$	$2\times4c$
II Maximal *klassengleiche* subgroups				
Enlarged unit cell, isomorphic				
[3] $Fdd2$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x+\frac{1}{4}, y+\frac{1}{4}, z; \pm(\frac{1}{3}, 0, 0)$	$8a; 16b$	$3\times16b$
[5] $Fdd2$	$5\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{5}x, y, z; \pm(\frac{1}{5}, 0, 0); \pm(\frac{2}{5}, 0, 0)$	$8a; 2\times16b$	$5\times16b$
[p] $Fdd2$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x+s, y+s, z; +(\frac{u}{p}, 0, 0)$	$8a; \frac{p-1}{2}\times16b$	$p\times16b$
	p = prime; $u = 1, \ldots, p-1$	$s = 0$ if $p = 4n+1$		
		$s = \frac{1}{4}$ if $p = 4n-1$		
[3] $Fdd2$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x+\frac{1}{4}, \frac{1}{3}y+\frac{1}{4}, z; \pm(0, \frac{1}{3}, 0)$	$8a; 16b$	$3\times16b$
[5] $Fdd2$	$\mathbf{a}, 5\mathbf{b}, \mathbf{c}$	$x, \frac{1}{5}y, z; \pm(0, \frac{1}{5}, 0); \pm(0, \frac{2}{5}, 0)$	$8a; 2\times16b$	$5\times16b$
[p] $Fdd2$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x+s, \frac{1}{p}y+s, z; +(0, \frac{u}{p}, 0)$	$8a; \frac{p-1}{2}\times16b$	$p\times16b$
	p = prime; $u = 1, \ldots, p-1$	$s = 0$ if $p = 4n+1$		
		$s = \frac{1}{4}$ if $p = 4n-1$		
[3] $Fdd2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3\times8a$	$3\times16b$
[5] $Fdd2$	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0, 0, \frac{1}{5}); \pm(0, 0, \frac{2}{5})$	$5\times8a$	$5\times16b$
[p] $Fdd2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x+s, y+s, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$p\times8a$	$p\times16b$
	p = prime; $u = 1, \ldots, p-1$	$s = 0$ if $p = 4n+1$		
		$s = \frac{1}{4}$ if $p = 4n-1$		

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$F2dd$	$A \to B$; $C \to A$	$c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Fd2d$	$A \to C$; $C \to B$	$c \to b$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

$Imm2$ No. 44 C_{2v}^{20}

	Axes	Coordinates	Wyckoff positions 2a	2b	4c	4d	8e
I Maximal *translationengleiche* subgroups							
[2] $Im11$ (8)			2a	2a	4b	2×2a	2×4b
≙ $I1m1$							
≙ $C1m1$	$-\mathbf{b}-\mathbf{c}, \mathbf{a}, \mathbf{c}$	$-y, x, -y+z$					
[2] $I1m1$ (8)			2a	2a	2×2a	4b	2×4b
[2] $I112$ (5)			2a	2b	4c	4c	2×4c
II Maximal *klassengleiche* subgroups							
Loss of centring translations							
[2] $Pnn2$ (34)			2a	2b	4c	4c	2×4c
[2] $Pmn2_1$ (31)		$x, y+\frac{1}{4}, z$	2a	2a	4b	2×2a	2×4b
[2] $Pnm2_1$ (31)		$x+\frac{1}{4}, y, z$	2a	2a	2×2a	4b	2×4b
≙ $Pmn2_1$	$\mathbf{b}, \mathbf{a}, -\mathbf{c}$	$y, x+\frac{1}{4}, -z$					
[2] $Pmm2$ (25)			1a; 1d	1b; 1c	2e; 2f	2g; 2h	2×4i
Enlarged unit cell, isomorphic							
[3] $Imm2$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	2a; 4c	2b; 4c	3×4c	4d; 8e	3×8e
[p] $Imm2$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	2a; $\frac{p-1}{2}$×4c	2b; $\frac{p-1}{2}$×4c	p×4c	4d; $\frac{p-1}{2}$×8e	p×8e
	p = prime > 2; $u = 1, \ldots, p-1$						
[3] $Imm2$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	2a; 4d	2b; 4d	4c; 8e	3×4d	3×8e
[p] $Imm2$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	2a; $\frac{p-1}{2}$×4d	2b; $\frac{p-1}{2}$×4d	4c; $\frac{p-1}{2}$×8e	p×4d	p×8e
	p = prime > 2; $u = 1, \ldots, p-1$						
[3] $Imm2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	3×2a	3×2b	3×4c	3×4d	3×8e
[p] $Imm2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	p×2a	p×2b	p×4c	p×4d	p×8e
	p = prime > 2; $u = 1, \ldots, p-1$						

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$I2mm$ $C \to A$ $\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$ $x \to y \to z \to x$

$Im2m$ $C \to B$ $\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$ $x \leftarrow y \leftarrow z \leftarrow x$

C_{2v}^{21} No. 45 $Iba2$

	Axes	Coordinates	Wyckoff positions 4a	4b	8c
I Maximal *translationengleiche* subgroups					
[2] $Ic11$ (9)			$4a$	$4a$	$2\times4a$
$\widehat{=}$ $I1a1$	**c**, **a**, **b**	z,x,y			
$\widehat{=}$ $C1c1$	−**b**−**c**, **a**, **c**	$-y,x,-y+z$			
[2] $I1c1$ (9)			$4a$	$4a$	$2\times4a$
$\widehat{=}$ $I1a1$		$x,y+\frac{1}{4},y$			
$\widehat{=}$ $C1c1$	**a**−**c**, **b**, **c**	$x,y,x+z$			
[2] $I112$ (5)			$2\times2a$	$2\times2b$	$2\times4c$
$\widehat{=}$ $A112$	**b**, −**a**−**b**, **c**	$x+y,-x,z$			
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $Pba2$ (32)			$2\times2a$	$2\times2b$	$2\times4c$
[2] $Pca2_1$ (29)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4a$	$4a$	$2\times4a$
[2] $Pbc2_1$ (29)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $Pca2_1$	**b**, **a**, −**c**	$y+\frac{1}{4},x+\frac{1}{4},-z$			
[2] $Pcc2$ (27)			$2a;2d$	$2b;2c$	$2\times4e$
Enlarged unit cell, isomorphic					
[3] $Iba2$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a;8c$	$4b;8c$	$3\times8c$
[p] $Iba2$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$4a;\frac{p-1}{2}\times8c$	$4b;\frac{p-1}{2}\times8c$	$p\times8c$
	p = prime >2; $u=1,\ldots,p-1$				
[3] $Iba2$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;8c$	$4b;8c$	$3\times8c$
[p] $Iba2$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$4a;\frac{p-1}{2}\times8c$	$4b;\frac{p-1}{2}\times8c$	$p\times8c$
	p = prime >2; $u=1,\ldots,p-1$				
[3] $Iba2$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times4a$	$3\times4b$	$3\times8c$
[p] $Iba2$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times4a$	$p\times4b$	$p\times8c$
	p = prime >2; $u=1,\ldots,p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$I2cb$	$A\to B$; $C\to A$	$a\to b\to c\to a$	**a** → **b** → **c** → **a**	$x\to y\to z\to x$
$Ic2a$	$A\to C$; $C\to B$	$a\leftarrow b\leftarrow c\leftarrow a$	**a** ← **b** ← **c** ← **a**	$x\leftarrow y\leftarrow z\leftarrow x$

*Ima*2 No. 46 C_{2v}^{22}

	Axes	Coordinates	Wyckoff positions 4*a*	4*b*	8*c*
I Maximal *translationengleiche* subgroups					
[2] *I*1*a*1 (9)			4*a*	4*a*	2×4*a*
$\widehat{=}$ *C*1*c*1	**−a−c**, **b**, **a**	$-z, y, x-z$			
[2] *Im*11 (8)		$x+\frac{1}{4}, y, z$	4*b*	2×2*a*	2×4*b*
$\widehat{=}$ *I*1*m*1	**c**, **a**, **b**	$z, x+\frac{1}{4}, y$			
$\widehat{=}$ *C*1*m*1	**−b−c**, **a**, **c**	$-y, x+\frac{1}{4}, -y+z$			
[2] *I*112 (5)			2*a*; 2*b*	4*c*	2×4*c*
$\widehat{=}$*A*112	**b**, **−a−b**, **c**	$-x+y, -x, z$			
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $Pna2_1$ (33)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	4*a*	4*a*	2×4*a*
[2] *Pnc*2 (30)			2*a*; 2*b*	4*c*	2×4*c*
[2] *Pma*2 (28)			2*a*; 2*b*	2×2*c*	2×4*d*
[2] $Pmc2_1$ (26)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	4*c*	2*a*; 2*b*	2×4*c*
Enlarged unit cell, isomorphic					
[3] *Ima*2	3**a**, **b**, **c**	$\frac{1}{3}x, y, z;\ \pm(\frac{1}{3}, 0, 0)$	4*a*; 8*c*	4*b*; 8*c*	3×8*c*
[*p*] *Ima*2	*p***a**, **b**, **c**	$\frac{1}{p}x, y, z;\ +(\frac{u}{p}, 0, 0)$	4*a*; $\frac{p-1}{2}$×8*c*	4*b*; $\frac{p-1}{2}$×8*c*	*p*×8*c*
	p = prime > 2; $u = 1, \ldots, p-1$				
[3] *Ima*2	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z;\ \pm(0, \frac{1}{3}, 0)$	4*a*; 8*c*	3×4*b*	3×8*c*
[*p*] *Ima*2	**a**, *p***b**, **c**	$x, \frac{1}{p}y, z;\ +(0, \frac{u}{p}, 0)$	4*a*; $\frac{p-1}{2}$×8*c*	*p*×4*b*	*p*×8*c*
	p = prime > 2; $u = 1, \ldots, p-1$				
[3] *Ima*2	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z;\ \pm(0, 0, \frac{1}{3})$	3×4*a*	3×4*b*	3×8*c*
[*p*] *Ima*2	**a**, **b**, *p***c**	$x, y, \frac{1}{p}y;\ +(0, 0, \frac{u}{p})$	*p*×4*a*	*p*×4*b*	*p*×8*c*
	p = prime > 2; $u = 1, \ldots, p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

*I*2*mb*	$A \to B;\ C \to A$	$a \to b;\ c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
*Ic*2*m*	$A \to C;\ C \to B$	$a \to c;\ c \to b$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
*Ibm*2	$A \to B$	$a \to b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
*I*2*cm*	$A \rightleftarrows C$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
*Im*2*a*	$C \to B$	$c \to b$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

D_{2h}^{1} $P2/m2/m2/m$ No. 47 $Pmmm$

	Axes	Coordinates	1a	1b	1c 2l	1d 2m	1e 2n 4u	1f 2o 4v	1g 2p 4w	1h 2q 4x	2i 2r 4y	2j 2s 4z	2k 2t 8α
I Maximal *translationengleiche* subgroups													
[2] *P*2*mm* (25) ≙*Pmm*2	 **b**, **c**, **a**	 y,z,x	1a	1a	1b 2×1d	1b 2e	1c 2f 4i	1c 2e 4i	1d 2f 2×2g	1d 2g 2×2h	2×1a 2h 2×2e	2×1b 2g 2×2f	2×1c 2h 2×4i
[2] *Pm*2*m* (25) ≙*Pmm*2	 **c**, **a**, **b**	 z,x,y	1a	1b	1c 2h	1d 2×1a	1a 2×1c 2×2e	1b 2×1b 2×2f	1c 2×1d 4i	1d 2e 4i	2g 2e 2×2g	2h 2f 2×2h	2g 2f 2×4i
[2] *Pmm*2 (25)			1a	1c	1a 2f	1c 2g	1b 2g 2×2g	1d 2h 2×2h	1b 2h 2×2e	1d 2×1a 2×2f	2e 2×1b 4i	2e 2×1c 4i	2f 2×1d 2×4i
[2] *P*222 (16)			1a	1b	1d 2l	1f 2m	1c 2n 4u	1e 2o 4u	1g 2p 4u	1h 2q 4u	2i 2s 4u	2j 2r 4u	2k 2t 2×4u
[2] *P*2/*m*11 (10) ≙*P*12/*m*1	 **c**, **a**, **b**	 z,x,y	1a	1b	1d 2l	1e 2m	1c 2m 2×2m	1f 2n 2×2n	1g 2n 4o	1h 2m 4o	2i 2m 4o	2j 2n 4o	2k 2n 2×4o
[2] *P*12/*m*1 (10)			1a	1d	1c 2n	1g 2i	1b 2k 4o	1e 2j 4o	1f 2l 2×2m	1h 2m 2×2n	2m 2n 4o	2m 2m 4o	2n 2n 2×4o
[2] *P*112/*m* (10)			1a	1c	1b 2n	1f 2m	1d 2n 4o	1g 2m 4o	1e 2n 4o	1h 2i 4o	2m 2j 2×2m	2n 2k 2×2n	2m 2l 2×4o
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**													
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z;+(\frac{1}{2},0,0)$	4a;4b	8g	8i 16l	8d 2×8h	8h 16m 2×16m	8e 16o 32p	8c 16k 2×16n	8f 2×8i 32p	2×8g 16m 2×16o	16n 16n 32p	16o 16j 2×32p
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z;$ $+(\frac{1}{2},0,0)$	8g	4a;4b	8d 16l	8i 16o	8e 16k 32p	8h 2×8h 2×16m	8f 16m 2×16n	8c 16n 32p	2×8g 16j 2×16o	16n 2×8i 32p	16o 16m 2×32p
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z;$ $+(\frac{1}{2},0,0)$	8h	8e	8c 16n	8f 2×8h	4a;4b 16m 2×16m	8g 16o 32p	8i 16k 32p	8d 16m 2×16n	16o 2×8i 2×16o	16l 16j 32p	2×8g 16n 2×32p
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4};$ $+(\frac{1}{2},0,0)$	8i	8d	4a;4b 16o	8g 16m	8c 2×8h 2×16m	8f 16k 32p	8h 16o 2×16n	8e 2×8i 32p	16n 16m 32p	2×8g 16n 2×16o	16l 16j 2×32p
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};$ $+(\frac{1}{2},0,0)$	8c	8f	8h 2×8g	8e 16m	8i 2×8h 2×16m	8d 16k 32p	4a;4b 16o 32p	8g 16m 2×16n	16l 2×8i 32p	16o 16j 2×16o	16n 16n 2×32p
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4};$ $+(\frac{1}{2},0,0)$	8d	8i	8g 16o	4a;4b 16k	8f 16o 32p	8c 16m 2×16m	8e 2×8h 2×16n	8h 16n 32p	16n 16j 32p	2×8g 2×8i 2×16o	16l 16m 2×32p

	Axes	Coordinates	Wyckoff positions $1a$	 $1b$	 $1c$ $2l$	 $1d$ $2m$	 $1e$ $2n$ $4u$	 $1f$ $2o$ $4v$	 $1g$ $2p$ $4w$	 $1h$ $2q$ $4x$	 $2i$ $2r$ $4y$	 $2j$ $2s$ $4z$	 $2k$ $2t$ 8α
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z;$ $+(\frac{1}{2},0,0)$	$8e$	$8h$	$8f$ $16n$	$8c$ $16o$	$8g$ $16k$ $32p$	$4a;4b$ $2\times8h$ $2\times16m$	$8d$ $16m$ $32p$	$8i$ $16j$ $2\times16n$	$16o$ $16n$ $2\times16o$	$16l$ $16m$ $32p$	$2\times8g$ $2\times8i$ $2\times32p$
[2] *Fmmm* (69)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4};$ $+(\frac{1}{2},0,0)$	$8f$	$8c$	$8e$ $2\times8g$	$8h$ $16k$	$8d$ $16o$ $32p$	$8i$ $16m$ $2\times16m$	$8g$ $2\times8h$ $32p$	$4a;4b$ $16j$ $2\times16n$	$16l$ $16n$ $32p$	$16o$ $16m$ $2\times16o$	$16n$ $2\times8i$ $2\times32p$
[2] *Aemm* (67) $\widehat{=}$*Cmme*	**a**, 2**b**, 2**c** 2**b**,2**c**,**a**	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y, \frac{1}{2}z, x; +(\frac{1}{2},0,0)$	$4c$	$4d$	$4g$ $8n$	$4g$ $8h$	$4a$ $8n$ $16o$	$4b$ $8i$ $16o$	$4e$ $8n$ $2\times8m$	$4f$ $8m$ $16o$	$8m$ $8j$ $16o$	$2\times4g$ $8m$ $2\times8n$	$8l$ $8k$ $2\times16o$
[2] *Aemm* (67) $\widehat{=}$*Cmme*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z, x; +(\frac{1}{2},0,0)$	$4a$	$4b$	$4e$ $2\times4g$	$4f$ $8h$	$4c$ $8n$ $16o$	$4d$ $8i$ $16o$	$4g$ $8n$ $16o$	$4g$ $8j$ $2\times8m$	$8l$ $8m$ $16o$	$8n$ $8k$ $2\times8n$	$8m$ $8m$ $2\times16o$
[2] *Aemm* (67) $\widehat{=}$*Cmme*	**a**,2**b**,2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}; +(0,\frac{1}{2},0)$ $\frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2},0,0)$	$4g$	$4g$	$4c$ $8l$	$4d$ $8n$	$4e$ $8h$ $16o$	$4f$ $8n$ $16o$	$4a$ $8i$ $2\times8m$	$4b$ $8m$ $16o$	$2\times4g$ $8j$ $2\times8n$	$8m$ $8m$ $16o$	$8n$ $8k$ $2\times16o$
[2] *Aemm* (67) $\widehat{=}$*Cmme*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(0,\frac{1}{2},0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2},0,0)$	$4e$	$4f$	$4a$ $8m$	$4b$ $8n$	$4g$ $8h$ $16o$	$4g$ $8n$ $16o$	$4c$ $8i$ $16o$	$4d$ $8j$ $2\times8m$	$8n$ $8m$ $2\times8n$	$8l$ $8k$ $16o$	$2\times4g$ $8m$ $2\times16o$
[2] *Bmem* (67) $\widehat{=}$*Cmme*	2**a**, **b**, 2**c** 2**c**, 2**a**, **b**	$\frac{1}{2}x, y, \frac{1}{2}z; +(\frac{1}{2},0,0)$ $\frac{1}{2}z, \frac{1}{2}x, y; +(0,\frac{1}{2},0)$	$4c$	$4g$	$4a$ $8k$	$4e$ $8m$	$4d$ $8l$ $16o$	$4g$ $2\times4g$ $2\times8n$	$4b$ $8n$ $16o$	$4f$ $8h$ $16o$	$8m$ $8i$ $2\times8m$	$8j$ $8n$ $16o$	$8m$ $8n$ $2\times16o$
[2] *Bmem* (67) $\widehat{=}$*Cmme*	2**a**, **b**, 2**c** 2**c**,2**a**,**b**	$\frac{1}{2}x+\frac{1}{4}, y, \frac{1}{2}z; +(\frac{1}{2},0,0)$ $\frac{1}{2}z, \frac{1}{2}x+\frac{1}{4}, y; +(0,\frac{1}{2},0)$	$4g$	$4c$	$4e$ $8k$	$4a$ $2\times4g$	$4g$ $8n$ $2\times8n$	$4d$ $8m$ $16o$	$4f$ $8l$ $16o$	$4b$ $8n$ $16o$	$8m$ $8n$ $2\times8m$	$8j$ $8h$ $16o$	$8m$ $8i$ $2\times16o$
[2] *Bmem* (67) $\widehat{=}$*Cmme*	2**a**, **b**, 2**c** 2**c**,2**a**,**b**	$\frac{1}{2}x, y, \frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2},0,0)$ $\frac{1}{2}z+\frac{1}{4}, \frac{1}{2}x, y; +(0,\frac{1}{2},0)$	$4a$	$4e$	$4c$ $8m$	$4g$ $8l$	$4b$ $8m$ $16o$	$4f$ $8n$ $2\times8n$	$4d$ $2\times4g$ $16o$	$4g$ $8h$ $16o$	$8j$ $8i$ $16o$	$8m$ $8n$ $2\times8m$	$8k$ $8n$ $2\times16o$
[2] *Bmem* (67) $\widehat{=}$*Cmme*	2**a**, **b**, 2**c** 2**c**,2**a**,**b**	$\frac{1}{2}x+\frac{1}{4}, y, \frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2},0,0)$ $\frac{1}{2}z+\frac{1}{4}, \frac{1}{2}x+\frac{1}{4}, y; +(0,\frac{1}{2},0)$	$4e$	$4a$	$4g$ $8m$	$4c$ $8n$	$4f$ $2\times4g$ $2\times8n$	$4b$ $8l$ $16o$	$4g$ $8m$ $16o$	$4d$ $8n$ $16o$	$8j$ $8n$ $16o$	$8m$ $8h$ $2\times8m$	$8k$ $8i$ $2\times16o$
[2] *Cmme* (67)	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0)$	$4c$	$4a$	$4d$ $8n$	$4b$ $8m$	$4g$ $8m$ $2\times8m$	$4e$ $8j$ $16o$	$4g$ $8k$ $16o$	$4f$ $8m$ $2\times8n$	$8h$ $2\times4g$ $16o$	$8i$ $8l$ $16o$	$8n$ $8n$ $2\times16o$
[2] *Cmme* (67)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y, z; +(\frac{1}{2},0,0)$	$4a$	$4c$	$4b$ $8n$	$4d$ $8j$	$4e$ $8k$ $16o$	$4g$ $8m$ $2\times8m$	$4f$ $8m$ $16o$	$4g$ $8l$ $2\times8n$	$8h$ $8n$ $16o$	$8i$ $8m$ $16o$	$8n$ $2\times4g$ $2\times16o$
[2] *Cmme* (67)	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y+\frac{1}{4}, z; +(\frac{1}{2},0,0)$	$4g$	$4e$	$4g$ $8i$	$4f$ $8m$	$4c$ $8m$ $2\times8m$	$4a$ $8j$ $16o$	$4d$ $8k$ $2\times8n$	$4b$ $2\times4g$ $16o$	$8n$ $8m$ $16o$	$8n$ $8n$ $16o$	$8h$ $8l$ $2\times16o$
[2] *Cmme* (67)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, z; +(\frac{1}{2},0,0)$	$4e$	$4g$	$4f$ $8i$	$4g$ $8j$	$4a$ $8k$ $16o$	$4c$ $8m$ $2\times8m$	$4b$ $8m$ $2\times8n$	$4d$ $8n$ $16o$	$8n$ $8l$ $16o$	$8n$ $2\times4g$ $16o$	$8h$ $8m$ $2\times16o$

	Axes	Coordinates	$1a$	$1b$	$1c$ $2l$	$1d$ $2m$	$1e$ $2n$ $4u$	$1f$ $2o$ $4v$	$1g$ $2p$ $4w$	$1h$ $2q$ $4x$	$2i$ $2r$ $4y$	$2j$ $2s$ $4z$	$2k$ $2t$ 8α
[2] *Ammm* (65) $\widehat{=}$*Cmmm*	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $2\mathbf{b}, 2\mathbf{c}, \mathbf{a}$	$x, \frac{1}{2}y, \frac{1}{2}z; +(0, \frac{1}{2}, 0)$ $\frac{1}{2}y, \frac{1}{2}z, x; +(\frac{1}{2}, 0, 0)$	$2a;2b$	$2c;2d$	$4i$ $8m$	$4j$ $2\times4g$	$4g$ $8p$ $2\times8p$	$4h$ $2\times4h$ $2\times8q$	$4e$ $8q$ $2\times8n$	$4f$ $2\times4i$ $16r$	$4k;4l$ $8p$ $2\times8o$	$8n$ $2\times4j$ $16r$	$8o$ $8q$ $2\times16r$
[2] *Ammm* (65) $\widehat{=}$*Cmmm*	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $2\mathbf{b}, 2\mathbf{c}, \mathbf{a}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0, \frac{1}{2}, 0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z, x; +(\frac{1}{2}, 0, 0)$	$4g$	$4h$	$4e$ $8n$	$4f$ $2\times4g$	$2a;2b$ $8p$ $2\times8p$	$2c;2d$ $2\times4h$ $2\times8q$	$4i$ $8q$ $16r$	$4j$ $8p$ $2\times8n$	$8o$ $2\times4i$ $2\times8o$	$8m$ $8q$ $16r$	$4k;4l$ $2\times4j$ $2\times16r$
[2] *Ammm* (65) $\widehat{=}$*Cmmm*	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $2\mathbf{b}, 2\mathbf{c}, \mathbf{a}$	$x, \frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}; +(0, \frac{1}{2}, 0)$ $\frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2}, 0, 0)$	$4i$	$4j$	$2a;2b$ $8o$	$2c;2d$ $8p$	$4e$ $2\times4g$ $2\times8p$	$4f$ $8q$ $2\times8q$	$4g$ $2\times4h$ $2\times8n$	$4h$ $2\times4i$ $16r$	$8n$ $8p$ $16r$	$4k;4l$ $2\times4j$ $2\times8o$	$8m$ $8q$ $2\times16r$
[2] *Ammm* (65) $\widehat{=}$*Cmmm*	$\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ $2\mathbf{b}, 2\mathbf{c}, \mathbf{a}$	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(0, \frac{1}{2}, 0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2}, 0, 0)$	$4e$	$4f$	$4g$ $4k;4l$	$4h$ $8p$	$4i$ $2\times4g$ $2\times8p$	$4j$ $8q$ $2\times8q$	$2a;2b$ $2\times4h$ $16r$	$2c;2d$ $8p$ $2\times8n$	$8m$ $2\times4i$ $16r$	$8o$ $8q$ $2\times8o$	$8n$ $2\times4j$ $2\times16r$
[2] *Bmmm* (65) $\widehat{=}$*Cmmm*	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ $2\mathbf{c}, 2\mathbf{a}, \mathbf{b}$	$\frac{1}{2}x, y, \frac{1}{2}z; +(\frac{1}{2}, 0, 0)$ $\frac{1}{2}z, \frac{1}{2}x, y; +(0, \frac{1}{2}, 0)$	$2a;2b$	$4i$	$4g$ $8q$	$4e$ $4k;4l$	$2c;2d$ $8o$ $2\times8o$	$4j$ $8n$ $16r$	$4h$ $8m$ $2\times8p$	$4f$ $2\times4g$ $2\times8q$	$2\times4i$ $2\times4h$ $2\times8n$	$8p$ $8p$ $16r$	$2\times4j$ $8q$ $2\times16r$
[2] *Bmmm* (65) $\widehat{=}$*Cmmm*	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ $2\mathbf{c}, 2\mathbf{a}, \mathbf{b}$	$\frac{1}{2}x+\frac{1}{4}, y, \frac{1}{2}z; +(\frac{1}{2}, 0, 0)$ $\frac{1}{2}z, \frac{1}{2}x+\frac{1}{4}, y; +(0, \frac{1}{2}, 0)$	$4i$	$2a;2b$	$4e$ $8q$	$4g$ $8n$	$4j$ $8m$ $16r$	$2c;2d$ $4k;4l$ $2\times8o$	$4f$ $8o$ $2\times8p$	$4h$ $8p$ $2\times8q$	$2\times4i$ $8q$ $2\times8n$	$8p$ $2\times4g$ $16r$	$2\times4j$ $2\times4h$ $2\times16r$
[2] *Bmmm* (65) $\widehat{=}$*Cmmm*	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ $2\mathbf{c}, 2\mathbf{a}, \mathbf{b}$	$\frac{1}{2}x, y, \frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2}, 0, 0)$ $\frac{1}{2}z+\frac{1}{4}, \frac{1}{2}x, y; +(0, \frac{1}{2}, 0)$	$4g$	$4e$	$2a;2b$ $2\times4j$	$4i$ $8o$	$4h$ $4k;4l$ $2\times8o$	$4f$ $8m$ $16r$	$2c;2d$ $8n$ $2\times8p$	$4j$ $2\times4g$ $2\times8q$	$8p$ $2\times4h$ $16r$	$2\times4i$ $8p$ $2\times8n$	$8q$ $8q$ $2\times16r$
[2] *Bmmm* (65) $\widehat{=}$*Cmmm*	$2\mathbf{a}, \mathbf{b}, 2\mathbf{c}$ $2\mathbf{c}, 2\mathbf{a}, \mathbf{b}$	$\frac{1}{2}x+\frac{1}{4}, y, \frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2}, 0, 0)$ $\frac{1}{2}z+\frac{1}{4}, \frac{1}{2}x+\frac{1}{4}, y; +(0, \frac{1}{2}, 0)$	$4e$	$4g$	$4i$ $2\times4j$	$2a;2b$ $8m$	$4f$ $8n$ $16r$	$4h$ $8o$ $2\times8o$	$4j$ $4k;4l$ $2\times8p$	$2c;2d$ $8p$ $2\times8q$	$8p$ $8q$ $16r$	$2\times4i$ $2\times4g$ $2\times8n$	$8q$ $2\times4h$ $2\times16r$
[2] *Cmmm* (65)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0)$	$2a;2b$	$4g$	$2c;2d$ $8q$	$4h$ $2\times4i$	$4i$ $2\times4j$ $2\times8n$	$4e$ $8p$ $16r$	$4j$ $8q$ $2\times8o$	$4f$ $4k;4l$ $16r$	$2\times4g$ $8n$ $2\times8p$	$2\times4h$ $8o$ $2\times8q$	$8p$ $8m$ $2\times16r$
[2] *Cmmm* (65)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0)$	$4g$	$2a;2b$	$4h$ $8q$	$2c;2d$ $8p$	$4e$ $8q$ $16r$	$4i$ $2\times4i$ $2\times8n$	$4f$ $2\times4j$ $2\times8o$	$4j$ $8o$ $16r$	$2\times4g$ $8m$ $2\times8p$	$2\times4h$ $4k;4l$ $2\times8q$	$8p$ $8n$ $2\times16r$
[2] *Cmmm* (65)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y+\frac{1}{4}, z; +(\frac{1}{2}, 0, 0)$	$4i$	$4e$	$4j$ $2\times4h$	$4f$ $2\times4i$	$2a;2b$ $2\times4j$ $2\times8n$	$4g$ $8p$ $16r$	$2c;2d$ $8q$ $16r$	$4h$ $8n$ $2\times8o$	$8p$ $4k;4l$ $2\times8p$	$8q$ $8m$ $2\times8q$	$2\times4g$ $8o$ $2\times16r$
[2] *Cmmm* (65)	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, z; +(\frac{1}{2}, 0, 0)$	$4e$	$4i$	$4f$ $2\times4h$	$4j$ $8p$	$4g$ $8q$ $16r$	$2a;2b$ $2\times4i$ $2\times8n$	$4h$ $2\times4j$ $16r$	$2c;2d$ $8m$ $2\times8o$	$8p$ $8o$ $2\times8p$	$8q$ $8n$ $2\times8q$	$2\times4g$ $4k;4l$ $2\times16r$
[2] *Pmma* (51)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$	$2a$	$2e$	$2c$ $4j$	$2e$ $4g$	$2b$ $4h$ $8l$	$2f$ $4k$ $2\times4k$	$2d$ $4k$ $2\times4i$	$2f$ $4i$ $2\times4j$	$4i$ $4j$ $8l$	$4i$ $2\times2e$ $8l$	$4j$ $2\times2f$ $2\times8l$
[2] *Pmma* (51)	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, y, z;\ +(\frac{1}{2}, 0, 0)$	$2e$	$2a$	$2e$ $4j$	$2c$ $4k$	$2f$ $4k$ $2\times4k$	$2b$ $4g$ $8l$	$2f$ $4h$ $2\times4i$	$2d$ $2\times2e$ $2\times4j$	$4i$ $2\times2f$ $8l$	$4i$ $4i$ $8l$	$4j$ $4j$ $2\times8l$
[2] *Pmam* (51) $\widehat{=}$*Pmma*	$2\mathbf{a}, \mathbf{b}, \mathbf{c}$ $2\mathbf{a}, -\mathbf{c}, \mathbf{b}$	$\frac{1}{2}x, y, z;\ +(\frac{1}{2}, 0, 0)$ $\frac{1}{2}x, -z, y\ +(\frac{1}{2}, 0, 0)$	$2a$	$2e$	$2b$ $4j$	$2f$ $4i$	$2c$ $4j$ $8l$	$2e$ $2\times2e$ $2\times4k$	$2d$ $2\times2f$ $8l$	$2f$ $4g$ $8l$	$4i$ $4h$ $2\times4i$	$4j$ $4k$ $2\times4j$	$4i$ $4k$ $2\times8l$

	Axes	Coordinates	1*a*	1*b*	1*c*	1*d* 2*m*	1*e* 2*n*	1*f* 2*o*	1*g* 2*p* 4*v*	1*h* 2*q* 4*w*	2*i* 2*r* 4*x*	2*j* 2*s* 4*y*	2*k* 2*t* 4*z*	2*l* 4*u* 8*α*
[2] *Pmam*	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	2*e*	2*a*	2*f*	2*b*	2*e*	2*c*	2*f*	2*d*	4*i*	4*j*	4*i*	4*j*
(51)						2×2*e*	2×2*f*	4*i*	4*j*	4*k*	4*k*	4*g*	4*h*	2×4*k*
≙ *Pmma*	2**a**, −**c**, **b**	$\frac{1}{2}x+\frac{1}{4},-z,y+(\frac{1}{2},0,0)$							8*l*	8*l*	8*l*	2×4*i*	2×4*j*	2×8*l*
[2] *Pbmm*	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2*a*	2*c*	2*b*	2*d*	2*e*	2*e*	2*f*	2*f*	4*i*	4*j*	2×2*e*	2×2*f*
(51)						4*i*	4*j*	4*i*	4*j*	4*g*	4*k*	4*h*	4*k*	8*l*
≙ *Pmma*	2**b**, **c**, **a**	$\frac{1}{2}y,z,x;\ +(\frac{1}{2},0,0)$							8*l*	8*l*	2×4*k*	2×4*i*	2×4*j*	2×8*l*
[2] *Pbmm*	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	2*e*	2*e*	2*f*	2*f*	2*a*	2*c*	2*b*	2*d*	2×2*e*	2×2*f*	4*i*	4*j*
(51)						4*i*	4*j*	4*i*	4*j*	4*k*	4*g*	4*k*	4*h*	8*l*
≙ *Pmma*	2**b**, **c**, **a**	$\frac{1}{2}y+\frac{1}{4},z,x;\ +(\frac{1}{2},0,0)$							8*l*	2×4*k*	8*l*	2×4*i*	2×4*j*	2×8*l*
[2] *Pmmb*	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2*a*	2*b*	2*c*	2*d*	2*e*	2*f*	2*e*	2*f*	4*g*	4*h*	4*k*	4*k*
(51)						4*i*	4*i*	4*j*	4*j*	4*i*	2×2*e*	4*j*	2×2*f*	2×4*i*
≙ *Pmma*	2**b**, −**a**, **c**	$\frac{1}{2}y,-x,z;\ +(\frac{1}{2},0,0)$							2×4*j*	8*l*	2×4*k*	8*l*	8*l*	2×8*l*
[2] *Pmmb*	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	2*e*	2*f*	2*e*	2*f*	2*a*	2*b*	2*c*	2*d*	4*k*	4*k*	4*g*	4*h*
(51)						4*i*	4*i*	4*j*	4*j*	2×2*e*	4*i*	2×2*f*	4*j*	2×4*i*
≙ *Pmma*	2**b**, −**a**, **c**	$\frac{1}{2}y+\frac{1}{4},-x,z;\ +(\frac{1}{2},0,0)$							2×4*j*	2×4*k*	8*l*	8*l*	8*l*	2×8*l*
[2] *Pcmm*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2*a*	2*c*	2*e*	2*e*	2*b*	2*d*	2*f*	2*f*	4*i*	2×2*e*	4*j*	2×2*f*
(51)						4*g*	4*k*	4*h*	4*k*	4*i*	4*j*	4*i*	4*j*	8*l*
≙ *Pmma*	2**c**, −**b**, **a**	$\frac{1}{2}z,-y,x;\ +(\frac{1}{2},0,0)$							8*l*	2×4*i*	2×4*j*	8*l*	2×4*k*	2×8*l*
[2] *Pcmm*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	2*e*	2*e*	2*a*	2*c*	2*f*	2*f*	2*b*	2*d*	2×2*e*	4*i*	2×2*f*	4*j*
(51)						4*k*	4*g*	4*k*	4*h*	4*i*	4*j*	4*i*	4*j*	8*l*
≙ *Pmma*	2**c**, −**b**, **a**	$\frac{1}{2}z+\frac{1}{4},-y,x;\ +(\frac{1}{2},0,0)$							8*l*	2×4*i*	2×4*j*	2×4*k*	8*l*	2×8*l*
[2] *Pmcm*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2*a*	2*b*	2*e*	2*f*	2*c*	2*d*	2*e*	2*f*	4*g*	4*k*	4*h*	4*k*
(51)						4*i*	2×2*e*	4*j*	2×2*f*	4*i*	4*i*	4*j*	4*j*	2×4*i*
≙ *Pmma*	2**c**, **a**, **b**	$\frac{1}{2}z,x,y;\ +(\frac{1}{2},0,0)$							2×4*j*	8*l*	8*l*	8*l*	2×4*k*	2×8*l*
[2] *Pmcm*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	2*e*	2*f*	2*a*	2*b*	2*e*	2*f*	2*c*	2*d*	4*k*	4*g*	4*k*	4*h*
(51)						2×2*e*	4*i*	2×2*f*	4*j*	4*i*	4*i*	4*j*	4*j*	2×4*i*
≙ *Pmma*	2**c**, **a**, **b**	$\frac{1}{2}z+\frac{1}{4},x,y;\ +(\frac{1}{2},0,0)$							2×4*j*	8*l*	8*l*	2×4*k*	8*l*	2×8*l*
[2] *Pmaa*	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;\ +(\frac{1}{2},0,0)$	2*a*	2*e*	2*c*	2*g*	2*d*	2*f*	2*b*	2*h*	4*m*	4*o*	4*p*	4*n*
(49)						4*q*	4*q*	4*i*	4*j*	4*q*	4*q*	4*k*	4*l*	2×4*q*
≙ *Pccm*	**b**, **c**, 2**a**	$y,z,\frac{1}{2}x;\ +(0,0,\frac{1}{2})$							8*r*	8*r*	8*r*	8*r*	8*r*	2×8*r*
[2] *Pmaa*	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;\ +(\frac{1}{2},0,0)$	2*e*	2*a*	2*g*	2*c*	2*f*	2*d*	2*h*	2*b*	4*m*	4*o*	4*p*	4*n*
(49)						4*i*	4*j*	4*q*	4*q*	4*k*	4*l*	4*q*	4*q*	8*r*
≙ *Pccm*	**b**, **c**, 2**a**	$y,z,\frac{1}{2}x+\frac{1}{4};\ +(0,0,\frac{1}{2})$							2×4*q*	8*r*	8*r*	8*r*	8*r*	2×8*r*
[2] *Pbmb*	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2*a*	2*c*	2*d*	2*b*	2*e*	2*g*	2*f*	2*h*	4*q*	4*q*	4*k*	4*l*
(49)						4*m*	4*p*	4*o*	4*n*	4*q*	4*i*	4*q*	4*j*	8*r*
≙ *Pccm*	**c**, **a**, 2**b**	$z,x,\frac{1}{2}y;\ +(0,0,\frac{1}{2})$							8*r*	2×4*q*	8*r*	8*r*	8*r*	2×8*r*
[2] *Pbmb*	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	2*e*	2*g*	2*f*	2*h*	2*a*	2*c*	2*d*	2*b*	4*k*	4*l*	4*q*	4*q*
(49)						4*m*	4*p*	4*o*	4*n*	4*i*	4*q*	4*j*	4*q*	8*r*
≙ *Pccm*	**c**, **a**, 2**b**	$z,x,\frac{1}{2}y+\frac{1}{4};\ +(0,0,\frac{1}{2})$							8*r*	8*r*	2×4*q*	8*r*	8*r*	2×8*r*
[2] *Pccm*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	2*a*	2*d*	2*e*	2*f*	2*c*	2*b*	2*g*	2*h*	4*q*	4*i*	4*q*	4*j*
(49)						4*q*	4*k*	4*q*	4*l*	4*m*	4*o*	4*p*	4*n*	8*r*
									8*r*	8*r*	8*r*	2×4*q*	8*r*	2×8*r*
[2] *Pccm*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	2*e*	2*f*	2*a*	2*d*	2*g*	2*h*	2*c*	2*b*	4*i*	4*q*	4*j*	4*q*
(49)						4*k*	4*q*	4*l*	4*q*	4*m*	4*o*	4*p*	4*n*	8*r*
									8*r*	8*r*	8*r*	8*r*	2×4*q*	2×8*r*

	Axes	Coordinates	$1a$	$1b$ $2k$	$1c$ $2l$ $2t$	$1d$ $2m$ $4u$	$1e$ $2n$ $4v$	$1f$ $2o$ $4w$	$1g$ $2p$ $4x$	$1h$ $2q$ $4y$	$2i$ $2r$ $4z$	$2j$ $2s$ 8α
Enlarged unit cell, isomorphic												
[2] $Pmmm$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,y,z$; $+(\frac{1}{2},0,0)$	$1a;1b$	$2i$ $2\times 2k$	$1c;1d$ $2\times 2l$ $4x$	$2j$ $2m;2o$ $4u;4v$	$1e;1f$ $2n;2p$ 8α	$2k$ $4y$ $2\times 4w$	$1g;1h$ $4z$ $2\times 4x$	$2l$ $2q;2s$ $2\times 4y$	$2\times 2i$ $2r;2t$ $2\times 4z$	$2\times 2j$ $4w$ $2\times 8\alpha$
[2] $Pmmm$	$2\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},y,z$; $+(\frac{1}{2},0,0)$	$2i$	$1a;1b$ $2\times 2k$	$2j$ $2\times 2l$ $2r;2t$	$1c;1d$ $4y$ 8α	$2k$ $4z$ $4u;4v$	$1e;1f$ $2m;2o$ $2\times 4w$	$2l$ $2n;2p$ $2\times 4x$	$1g;1h$ $4w$ $2\times 4y$	$2\times 2i$ $4x$ $2\times 4z$	$2\times 2j$ $2q;2s$ $2\times 8\alpha$
[3] $Pmmm$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$1a;2i$	$1b;2i$ $3\times 2k$	$1c;2j$ $3\times 2l$ $2t;4x$	$1d;2j$ $2m;4y$ $4u;8\alpha$	$1e;2k$ $2n;4z$ $4v;8\alpha$	$1f;2k$ $2o;4y$ $3\times 4w$	$1g;2l$ $2p;4z$ $3\times 4x$	$1h;2l$ $2q;4w$ $3\times 4y$	$3\times 2i$ $2r;4x$ $3\times 4z$	$3\times 2j$ $2s;4w$ $3\times 8\alpha$
[p] $Pmmm$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$ p = prime >2; $u=1,\ldots,p-1$	$1a$; $\frac{p-1}{2}\times 2i$	$1b$; $\frac{p-1}{2}\times 2i$ $p\times 2k$	$1c$; $\frac{p-1}{2}\times 2j$ $p\times 2l$ $2t$; $\frac{p-1}{2}\times 4x$	$1d$; $\frac{p-1}{2}\times 2j$ $2m$; $\frac{p-1}{2}\times 4y$ $4u$; $\frac{p-1}{2}\times 8\alpha$	$1e$; $\frac{p-1}{2}\times 2k$ $2n$; $\frac{p-1}{2}\times 4z$ $4v$; $\frac{p-1}{2}\times 8\alpha$	$1f$; $\frac{p-1}{2}\times 2k$ $2o$; $\frac{p-1}{2}\times 4y$ $p\times 4w$	$1g$; $\frac{p-1}{2}\times 2l$ $2p$; $\frac{p-1}{2}\times 4z$ $p\times 4x$	$1h$; $\frac{p-1}{2}\times 2l$ $2q$; $\frac{p-1}{2}\times 4w$ $p\times 4y$	$p\times 2i$ $2r$; $\frac{p-1}{2}\times 4x$ $p\times 4z$	$p\times 2j$ $2s$; $\frac{p-1}{2}\times 4w$ $p\times 8\alpha$
[2] $Pmmm$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z$; $+(0,\frac{1}{2},0)$	$1a;1e$	$1b;1f$ $4y$	$1c;1g$ $4z$ $4v$	$1d;1h$ $2\times 2m$ $2\times 4u$	$2m$ $2\times 2n$ $2\times 4v$	$2o$ $2\times 2o$ $4w;4x$	$2n$ $2\times 2p$ 8α	$2p$ $2q;2r$ $2\times 4y$	$2i;2k$ $4u$ $2\times 4z$	$2j;2l$ $2s;2t$ $2\times 8\alpha$
[2] $Pmmm$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z$; $+(0,\frac{1}{2},0)$	$2m$	$2o$ $2i;2k$	$2n$ $2j;2l$ $2s;2t$	$2p$ $2\times 2m$ $2\times 4u$	$1a;1e$ $2\times 2n$ $2\times 4v$	$1b;1f$ $2\times 2o$ 8α	$1c;1g$ $2\times 2p$ $4w;4x$	$1d;1h$ $4u$ $2\times 4y$	$4y$ $2q;2r$ $2\times 4z$	$4z$ $4v$ $2\times 8\alpha$
[3] $Pmmm$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$1a;2m$	$1b;2o$ $2k;4y$	$1c;2n$ $2l;4z$ $2t;4v$	$1d;2p$ $3\times 2m$ $3\times 4u$	$1e;2m$ $3\times 2n$ $3\times 4v$	$1f;2o$ $3\times 2o$ $4w;8\alpha$	$1g;2n$ $3\times 2p$ $4x;8\alpha$	$1h;2p$ $2q;4u$ $3\times 4y$	$2i;4y$ $2r;4u$ $3\times 4z$	$2j;4z$ $2s;4v$ $3\times 8\alpha$
[p] $Pmmm$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$ p = prime >2; $u=1,\ldots,p-1$	$1a$; $\frac{p-1}{2}\times 2m$	$1b$; $\frac{p-1}{2}\times 2o$ $2k$; $\frac{p-1}{2}\times 4y$	$1c$; $\frac{p-1}{2}\times 2n$ $2l$; $\frac{p-1}{2}\times 4z$ $2t$; $\frac{p-1}{2}\times 4v$	$1d$; $\frac{p-1}{2}\times 2p$ $p\times 2m$ $p\times 4u$	$1e$; $\frac{p-1}{2}\times 2m$ $p\times 2n$ $p\times 4v$	$1f$; $\frac{p-1}{2}\times 2o$ $p\times 2o$ $4w$; $\frac{p-1}{2}\times 8\alpha$	$1g$; $\frac{p-1}{2}\times 2n$ $p\times 2p$ $4x$; $\frac{p-1}{2}\times 8\alpha$	$1h$; $\frac{p-1}{2}\times 2p$ $2q$; $\frac{p-1}{2}\times 4u$ $p\times 4y$	$2i$; $\frac{p-1}{2}\times 4y$ $2r$; $\frac{p-1}{2}\times 4u$ $p\times 4z$	$2j$; $\frac{p-1}{2}\times 4z$ $2s$; $\frac{p-1}{2}\times 4v$ $p\times 8\alpha$
[2] $Pmmm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a;1c$	$1b;1d$ $2k;2l$	$2q$ $4x$ $2\times 2t$	$2s$ $2m;2n$ $2\times 4u$	$1e;1g$ $4u$ $2\times 4v$	$1f;1h$ $2o;2p$ $2\times 4w$	$2r$ $4v$ $2\times 4x$	$2t$ $2\times 2q$ $4y;4z$	$2i;2j$ $2\times 2r$ 8α	$4w$ $2\times 2s$ $2\times 8\alpha$
[2] $Pmmm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2q$	$2s$ $4x$	$1a;1c$ $2k;2l$ $2\times 2t$	$1b;1d$ $4u$ $2\times 4u$	$2r$ $2m;2n$ $2\times 4v$	$2t$ $4v$ $2\times 4w$	$1e;1g$ $2o;2p$ $2\times 4x$	$1f;1h$ $2\times 2q$ 8α	$4w$ $2\times 2r$ $4y;4z$	$2i;2j$ $2\times 2s$ $2\times 8\alpha$
[3] $Pmmm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a;2q$	$1b;2s$ $2k;4x$	$1c;2q$ $2l;4x$ $3\times 2t$	$1d;2s$ $2m;4u$ $3\times 4u$	$1e;2r$ $2n;4u$ $3\times 4v$	$1f;2t$ $2o;4v$ $3\times 4w$	$1g;2r$ $2p;4v$ $3\times 4x$	$1h;2t$ $3\times 2q$ $4y;8\alpha$	$2i;4w$ $3\times 2r$ $4z;8\alpha$	$2j;4w$ $3\times 2s$ $3\times 8\alpha$
[p] $Pmmm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime >2; $u=1,\ldots,p-1$	$1a$; $\frac{p-1}{2}\times 2q$	$1b$; $\frac{p-1}{2}\times 2s$ $2k$; $\frac{p-1}{2}\times 4x$	$1c$; $\frac{p-1}{2}\times 2q$ $2l$; $\frac{p-1}{2}\times 4x$ $p\times 2t$	$1d$; $\frac{p-1}{2}\times 2s$ $2m$; $\frac{p-1}{2}\times 4u$ $p\times 4u$	$1e$; $\frac{p-1}{2}\times 2r$ $2n$; $\frac{p-1}{2}\times 4u$ $p\times 4v$	$1f$; $\frac{p-1}{2}\times 2t$ $2o$; $\frac{p-1}{2}\times 4v$ $p\times 4w$	$1g$; $\frac{p-1}{2}\times 2r$ $2p$; $\frac{p-1}{2}\times 4v$ $p\times 4x$	$1h$; $\frac{p-1}{2}\times 2t$ $p\times 2q$ $4y$; $\frac{p-1}{2}\times 4\alpha$	$2i$; $\frac{p-1}{2}\times 4w$ $p\times 2r$ $4z$; $\frac{p-1}{2}\times 4\alpha$	$2j$; $\frac{p-1}{2}\times 4w$ $p\times 2s$ $p\times 8\alpha$

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$Pnnn$ No. 48 $P2/n2/n2/n$ D_{2h}^{2}

	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$2c$	$2d$ $4i$	$4e$ $4j$	$4f$ $4k$	$4g$ $4l$	$4h$ $8m$
I Maximal *translationengleiche* subgroups											
[2] $P2nn$ (34) $\widehat{=}$ $Pnn2$	 **b**, **c**, **a**	 y,z,x	$x,y+\frac{1}{4},z+\frac{1}{4}$ $y+\frac{1}{4},z+\frac{1}{4},x$	$2a$	$2a$	$2b$	$2b$ $4c$	$4c$ $4c$	$4c$ $4c$	$2{\times}2a$ $4c$	$2{\times}2b$ $2{\times}4c$
[2] $Pn2n$ (34) $\widehat{=}$ $Pnn2$	 **c**, **a**, **b**	 z,x,y	$x+\frac{1}{4},y,z+\frac{1}{4}$ $z+\frac{1}{4},x+\frac{1}{4},y$	$2a$	$2b$	$2b$	$2a$ $2{\times}2a$	$4c$ $2{\times}2b$	$4c$ $4c$	$4c$ $4c$	$4c$ $2{\times}4c$
[2] $Pnn2$ (34)			$x+\frac{1}{4},y+\frac{1}{4},z$	$2a$	$2b$	$2a$	$2b$ $4c$	$4c$ $4c$	$4c$ $2{\times}2a$	$4c$ $2{\times}2b$	$4c$ $2{\times}4c$
[2] $P222$ (16)			$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$1a;1h$	$1b;1g$	$1d;1e$	$1c;1f$ $2m;2p$	$4u$ $2n;2o$	$4u$ $2q;2t$	$2i;2l$ $2r;2s$	$2j;2k$ $2{\times}4u$
[2] $P2/n11$ (13) $\widehat{=}$ $P12/n1$	 **c**, **a**, **b**	$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$ $z+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$	 z,x,y	$2e$	$2e$	$2f$	$2f$ $4g$	$2c;2d$ $4g$	$2a;2b$ $4g$	$2{\times}2e$ $4g$	$2{\times}2f$ $2{\times}4g$
[2] $P12/n1$ (13)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$		$2e$	$2f$	$2f$	$2e$ $2{\times}2e$	$2c;2d$ $2{\times}2f$	$2a;2b$ $4g$	$4g$ $4g$	$4g$ $2{\times}4g$
[2] $P112/n$ (13)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$		$2e$	$2f$	$2e$	$2f$ $4g$	$2c;2d$ $4g$	$2a;2b$ $2{\times}2e$	$4g$ $2{\times}2f$	$4g$ $2{\times}4g$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**											
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z$;	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$8a;8b$	$16e$	$16g$	$16f$ $2{\times}16f$	$16c;16d$ $32h$	$32h$ $2{\times}16g$	$2{\times}16e$ $32h$	$32h$ $2{\times}32h$
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z$;	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$16e$	$8a;8b$	$16f$	$16g$ $32h$	$32h$ $2{\times}16f$	$16c;16d$ $32h$	$2{\times}16e$ $2{\times}16g$	$32h$ $2{\times}32h$
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z$;	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$16f$	$16g$	$16e$	$8a;8b$ $2{\times}16f$	$32h$ $32h$	$16c;16d$ $32h$	$32h$ $2{\times}16g$	$2{\times}16e$ $2{\times}32h$
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4}$;	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$16g$	$16f$	$8a;8b$	$16e$ $32h$	$32h$ $2{\times}16f$	$16c;16d$ $2{\times}16g$	$32h$ $32h$	$2{\times}16e$ $2{\times}32h$
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$;	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$16e$	$8a;8b$	$16f$	$16g$ $32h$	$16c;16d$ $2{\times}16f$	$32h$ $32h$	$2{\times}16e$ $2{\times}16g$	$32h$ $2{\times}32h$
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4}$;	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$16f$	$16g$	$16e$	$8a;8b$ $2{\times}16f$	$16c;16d$ $32h$	$32h$ $32h$	$32h$ $2{\times}16g$	$2{\times}16e$ $2{\times}32h$
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z$;	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$16g$	$16f$	$8a;8b$	$16e$ $32h$	$16c;16d$ $2{\times}16f$	$32h$ $2{\times}16g$	$32h$ $32h$	$2{\times}16e$ $2{\times}32h$
[2] $Fddd$ (70)	2**a**, 2**b**, 2**c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4}$, $\frac{1}{2}z+\frac{1}{4}$;	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$8a;8b$	$16e$	$16g$	$16f$ $2{\times}16f$	$32h$ $32h$	$16c;16d$ $2{\times}16g$	$2{\times}16e$ $32h$	$32h$ $2{\times}32h$

Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions $2a$	$2b$	$2c$	$2d$ $4i$	$4e$ $4j$	$4f$ $4k$	$4g$ $4l$	$4h$ $8m$
Enlarged unit cell, isomorphic										
[3] $Pnnn$ $3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$2a(b^*);4g$	$2b(a^*);4g$	$2c(d^*);4h$	$2d(c^*);4h$ $4i(j^*);8m$	$4f(e^*);8m$ $4j(i^*);8m$	$4e(f^*);8m$ $4k(l^*);8m$	$3\times 4g$ $4l(k^*);8m$	$3\times 4h$ $3\times 8m$
[p] $Pnnn$ $p\mathbf{a},\mathbf{b},\mathbf{c}$ $p=$ prime >2; $u=1,\ldots,p-1$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$	$2a(b^\dagger)$; $\frac{p-1}{2}\times 4g$	$2b(a^\dagger)$; $\frac{p-1}{2}\times 4g$	$2c(d^\dagger)$; $\frac{p-1}{2}\times 4h$	$2d(c^\dagger)$; $\frac{p-1}{2}\times 4h$ $4i(j^\dagger)$; $\frac{p-1}{2}\times 8m$	$4e(f^\ddagger)$; $\frac{p-1}{2}\times 8m$ $4j(i^\dagger)$; $\frac{p-1}{2}\times 8m$	$4f(e^\ddagger)$; $\frac{p-1}{2}\times 8m$ $4k(l^\dagger)$; $\frac{p-1}{2}\times 8m$	$p\times 4g$ $4l(k^\dagger)$; $\frac{p-1}{2}\times 8m$	$p\times 4h$ $p\times 8m$
[3] $Pnnn$ $\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$2a(d^*);4i$	$2b(c^*);4j$	$2c(b^*);4j$	$2d(a^*);4i$ $3\times 4i$	$4f(e^*);8m$ $3\times 4j$	$4e(f^*);8m$ $4k(l^*);8m$	$4g(h^*);8m$ $4l(k^*);8m$	$4h(g^*);8m$ $3\times 8m$
[p] $Pnnn$ $\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=$ prime >2; $u=1,\ldots,p-1$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	$2a(d^\dagger)$; $\frac{p-1}{2}\times 4i$	$2b(c^\dagger)$; $\frac{p-1}{2}\times 4j$	$2c(b^\dagger)$; $\frac{p-1}{2}\times 4j$	$2d(a^\dagger)$; $\frac{p-1}{2}\times 4i$ $p\times 4i$	$4e(f^\ddagger)$; $\frac{p-1}{2}\times 8m$ $p\times 4j$	$4f(e^\ddagger)$; $\frac{p-1}{2}\times 8m$ $4k(l^\dagger)$; $\frac{p-1}{2}\times 8m$	$4g(h^\dagger)$; $\frac{p-1}{2}\times 8m$ $4l(k^\dagger)$; $\frac{p-1}{2}\times 8m$	$4h(g^\dagger)$; $\frac{p-1}{2}\times 8m$ $p\times 8m$
[3] $Pnnn$ $\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a(c^*);4k$	$2b(d^*);4l$	$2c(a^*);4k$	$2d(b^*);4l$ $4i(j^*);8m$	$4f(e^*);8m$ $4j(i^*);8m$	$4e(f^*);8m$ $3\times 4k$	$4g(h^*);8m$ $3\times 4l$	$4h(g^*);8m$ $3\times 8m$
[p] $Pnnn$ $\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=$ prime >2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a(c^\dagger)$; $\frac{p-1}{2}\times 4k$	$2b(d^\dagger)$; $\frac{p-1}{2}\times 4l$	$2c(a^\dagger)$; $\frac{p-1}{2}\times 4k$	$2d(b^\dagger)$; $\frac{p-1}{2}\times 4l$ $4i(j^\dagger)$; $\frac{p-1}{2}\times 8m$	$4e(f^\ddagger)$; $\frac{p-1}{2}\times 8m$ $4j(i^\dagger)$; $\frac{p-1}{2}\times 8m$	$4f(e^\ddagger)$; $\frac{p-1}{2}\times 8m$ $p\times 4k$	$4g(h^\dagger)$; $\frac{p-1}{2}\times 8m$ $p\times 4l$	$4h(g^\dagger)$; $\frac{p-1}{2}\times 8m$ $p\times 8m$

* origin 2
† origin 2 and $p=4n-1$
‡ origin 1 and $p=4n-1$

Axes	Coordinates	Wyckoff positions $2a$	$2b$	$2c$	$2d$	$2e$ $4l$	$2f$ $4m$	$2g$ $4n$	$2h$ $4o$	$4i$ $4p$	$4j$ $4q$	$4k$ $8r$
[3] $Pccm$ $\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a;4m$	$2b;4n$	$2c;4o$	$2d;4p$	$2e;4m$ $4l;8r$	$2f;4p$ $3\times 4m$	$2g;4o$ $3\times 4n$	$2h;4n$ $3\times 4o$	$4i;8r$ $3\times 4p$	$4j;8r$ $4q;8r$	$4k;8r$ $3\times 8r$
[p] $Pccm$ $\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=$ prime >2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times 4m$	$2b$; $\frac{p-1}{2}\times 4n$	$2c$; $\frac{p-1}{2}\times 4o$	$2d$; $\frac{p-1}{2}\times 4p$	$2e$; $\frac{p-1}{2}\times 4m$ $4l$; $\frac{p-1}{2}\times 8r$	$2f$; $\frac{p-1}{2}\times 4p$ $p\times 4m$	$2g$; $\frac{p-1}{2}\times 4o$ $p\times 4n$	$2h$; $\frac{p-1}{2}\times 4n$ $p\times 4o$	$4i$; $\frac{p-1}{2}\times 8r$ $p\times 4p$	$4j$; $\frac{p-1}{2}\times 8r$ $4q$; $\frac{p-1}{2}\times 8r$	$4k$; $\frac{p-1}{2}\times 8r$ $p\times 8r$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pmaa$ $C\rightarrow A$ $a\rightarrow b\rightarrow c\rightarrow a$ $\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$ $x\rightarrow y\rightarrow z\rightarrow x$

$Pbmb$ $C\rightarrow B$ $a\leftarrow b\leftarrow c\leftarrow a$ $\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$ $x\leftarrow y\leftarrow z\leftarrow x$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 49, pp. 513–515.

Pccm No. 49 $P2/c\,2/c\,2/m$ D_{2h}^{3}

	Axes	Coordinates	Wyckoff positions										
			2a	2b	2c	2d	2e	2f	2g	2h	4i	4j	4k
							4l	4m	4n	4o	4p	4q	8r
I Maximal *translationengleiche* subgroups													
[2] *P*2*cm* (28)		$x,y,z+\frac{1}{4}$	2c	2c	2c	2c	2a	2a	2b	2b	2×2a	2×2b	4d
≙ *Pma*2	**c**, −**b**, **a**	$z+\frac{1}{4},-y,x$					4d	4d	4d	4d	4d	2×2c	2×4d
[2] *Pc*2*m* (28)		$x,y,z+\frac{1}{4}$	2c	2c	2c	2c	2a	2b	2a	2b	4d	4d	2×2a
≙ *Pma*2	**c**, **a**, **b**	$z+\frac{1}{4},x,y$					2×2b	4d	4d	4d	4d	2×2c	2×4d
[2] *Pcc*2 (27)			2a	2d	2b	2c	2a	2c	2b	2d	4e	4e	4e
							4e	2×2a	2×2d	2×2b	2×2c	4e	2×4e
[2] *P*222 (16)		$x,y,z+\frac{1}{4}$	2q	2t	2s	2r	1a; 1d	1b; 1f	1c; 1g	1e; 1h	2i; 2j	2k; 2l	2m; 2n
							2o; 2p	2×2q	2×2t	2×2s	2×2r	4u	2×4u
[2] *P*2/*c*11 (13)			2a	2b	2d	2c	2e	2e	2f	2f	2×2e	2×2f	4g
≙ *P*12/*c*1	−**b**, **a**, **c**	$-y,x,z$					4g	4g	4g	4g	4g	4g	2×4g
[2] *P*12/*c*1 (13)			2a	2b	2c	2d	2e	2f	2e	2f	4g	4g	2×2e
							2×2f	4g	4g	4g	4g	4g	2×4g
[2] *P*112/*m* (10)			1a; 1b	1g; 1h	1d; 1e	1c; 1f	2i	2k	2j	2l	4o	4o	4o
							4o	2×2i	2×2l	2×2j	2×2k	2m; 2n	2×4o
II Maximal *klassengleiche* subgroups													
Enlarged unit cell, non-isomorphic													
[2] *Ccce* (68)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z+\frac{1}{4};+(\frac{1}{2},0,0)$ (orig. 1)	8g	8h	8d	8c	4a; 4b	8e	8f	8h	2×8e	16i	2×8f
		origin 2: $\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$					16i	2×8g	2×8h	16i	16i	16i	2×16i
[2] *Ccce* (68)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z+\frac{1}{4};+(\frac{1}{2},0,0)$ (or. 1)	8c	8d	8h	8g	8e	4a; 4b	8h	8f	2×8e	16i	16i
		origin 2: $\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$					2×8f	16i	16i	2×8h	2×8g	16i	2×16i
[2] *Ccce* (68)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y-\frac{1}{4},z+\frac{1}{4};+(\frac{1}{2},0,0)$ (or. 1)	8d	8c	8g	8h	8f	8h	4a; 4b	8e	16i	2×8e	2×8f
		origin 2: $\frac{1}{2}x,\frac{1}{2}y,z;+(\frac{1}{2},0,0)$					16i	16i	16i	2×8g	2×8h	16i	2×16i
[2] *Ccce* (68)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y-\frac{1}{4},z+\frac{1}{4};+(\frac{1}{2},0,0)$	8h	8g	8c	8d	8h	8f	8e	4a; 4b	16i	2×8e	16i
		origin 2: $\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;+(\frac{1}{2},0,0)$ (or. 1)					2×8f	2×8h	2×8g	16i	16i	16i	2×16i
[2] *Cccm* (66)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z;+(\frac{1}{2},0,0)$	4c; 4d	4e; 4f	8l	8l	4a; 4b	8g	8h	8k	2×8g	16m	2×8h
							16m	8i; 8j	2×8k	16m	16m	2×8l	2×16m
[2] *Cccm* (66)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y,z;+(\frac{1}{2},0,0)$	8l	8l	4e; 4f	4c; 4d	8g	4a; 4b	8k	8h	2×8g	16m	16m
							2×8h	16m	16m	2×8k	8i; 8j	2×8l	2×16m
[2] *Cccm* (66)	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$	8l	8l	4c; 4d	4e; 4f	8h	8k	4a; 4b	8g	16m	2×8g	2×8h
							16m	16m	16m	8i; 8j	2×8k	2×8l	2×16m
[2] *Cccm* (66)	2**a**, 2**b**, **c**	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},z;+(\frac{1}{2},0,0)$	4e; 4f	4c; 4d	8l	8l	8k	8h	8g	4a; 4b	16m	2×8g	16m
							2×8h	2×8k	8i; 8j	16m	16m	2×8l	2×16m
[2] *Pcca* (54)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;+(\frac{1}{2},0,0)$	4a	4e	4b	4d	4c	4d	4c	4e	8f	8f	2×4c
							8f	8f	2×4e	8f	2×4d	8f	2×8f
[2] *Pcca* (54)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;+(\frac{1}{2},0,0)$	4d	4b	4e	4a	4d	4c	4e	4c	8f	8f	8f
							2×4c	2×4d	8f	2×4e	8f	8f	2×8f
[2] *Pccb* (54)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;+(0,\frac{1}{2},0)$	4a	4e	4d	4b	4c	4c	4d	4e	2×4c	8f	8f
≙ *Pcca*	2**b**, −**a**, **c**	$\frac{1}{2}y,-x,z;+(\frac{1}{2},0,0)$					8f	8f	2×4e	2×4d	8f	8f	2×8f
[2] *Pccb* (54)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;+(0,\frac{1}{2},0)$	4d	4b	4a	4e	4d	4e	4c	4c	8f	2×4c	8f
≙ *Pcca*	2**b**, −**a**, **c**	$\frac{1}{2}y+\frac{1}{4},-x,z;+(\frac{1}{2},0,0)$					8f	2×4d	8f	8f	2×4e	8f	2×8f
[2] *Pcnm* (53)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z;+(\frac{1}{2},0,0)$	2a; 2b	4h	2c; 2d	4h	4e	4g	4f	4g	8i	8i	8i
≙ *Pmna*	**c**, −**b**, 2**a**	$z,-y,\frac{1}{2}x;+(0,0,\frac{1}{2})$					2×4g	2×4e	8i	2×4f	8i	2×4h	2×8i
[2] *Pcnm* (53)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z;+(\frac{1}{2},0,0)$	4h	2c; 2d	4h	2a; 2b	4g	4e	4g	4f	8i	8i	2×4g
≙ *Pmna*	**c**, −**b**, 2**a**	$z,-y,\frac{1}{2}x+\frac{1}{4};+(0,0,\frac{1}{2})$					8i	8i	2×4f	8i	2×4e	2×4h	2×8i

	Axes	Coordinates	2*a*	2*b*	2*c*	2*d*	2*e* 4*l*	2*f* 4*m*	2*g* 4*n*	2*h* 4*o*	4*i* 4*p*	4*j* 4*q*	4*k* 8*r*
[2] *Pncm* (53) ≙ *Pmna*	**a**, 2**b**, **c** **c**, **a**, 2**b**	$x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$ $z, x, \frac{1}{2}y; +(0, 0, \frac{1}{2})$	2*a*;2*b*	4*h*	4*h*	2*c*;2*d*	4*e* 8*i*	4*f* 2×4*e*	4*g* 8*i*	4*g* 8*i*	8*i* 2×4*f*	2×4*g* 2×4*h*	8*i* 2×8*i*
[2] *Pncm* (53) ≙ *Pmna*	**a**, 2**b**, **c** **c**, **a**, 2**b**	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$ $z, x, \frac{1}{2}y+\frac{1}{4}; +(0, 0, \frac{1}{2})$	4*h*	2*c*;2*d*	2*a*;2*b*	4*h*	4*g* 8*i*	4*g* 8*i*	4*e* 2×4*f*	4*f* 2×4*e*	2×4*g* 8*i*	8*i* 2×4*h*	8*i* 2×8*i*
[2] *Pcna* (50) ≙ *Pban*	2**a**, **b**, **c** **c**, 2**a**, **b**	$\frac{1}{2}x+\frac{1}{4}, y, z+\frac{1}{4}; +(\frac{1}{2}, 0, 0)$ (or. 1) origin 2: $\frac{1}{2}x, y, z; +(\frac{1}{2}, 0, 0)$ $z+\frac{1}{4}, \frac{1}{2}x+\frac{1}{4}, y; +(0, \frac{1}{2}, 0)$ (or. 1) origin 2: $z, \frac{1}{2}x, y; +(0, \frac{1}{2}, 0)$	4*e*	4*h*	4*f*	4*g*	4*i* 4*k*;4*l*	2*a*;2*b* 8*m*	4*j* 2×4*h*	2*c*;2*d* 8*m*	2×4*i* 2×4*g*	2×4*j* 8*m*	8*m* 2×8*m*
[2] *Pcna* (50) ≙ *Pban*	2**a**, **b**, **c** **c**, 2**a**, **b**	$\frac{1}{2}x, y, z+\frac{1}{4}; +(\frac{1}{2}, 0, 0)$ (origin 1) origin 2: $\frac{1}{2}x+\frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$ $z+\frac{1}{4}, \frac{1}{2}x, y; +(0, \frac{1}{2}, 0)$ (origin 1) origin 2: $z, \frac{1}{2}x+\frac{1}{4}, y; +(0, \frac{1}{2}, 0)$	4*g*	4*f*	4*h*	4*e*	2*a*;2*b* 8*m*	4*i* 2×4*g*	2*c*;2*d* 8*m*	4*j* 2×4*h*	2×4*i* 8*m*	2×4*j* 8*m*	4*k*;4*l* 2×8*m*
[2] *Pncb* (50) ≙ *Pban*	**a**, 2**b**, **c** 2**b**, **c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, z+\frac{1}{4}; +(0, \frac{1}{2}, 0)$ (or. 1) origin 2: $x, \frac{1}{2}y, z; +(0, \frac{1}{2}, 0)$ $\frac{1}{2}y+\frac{1}{4}, z+\frac{1}{4}, x; +(\frac{1}{2}, 0, 0)$ (or. 1) $\frac{1}{2}y, z, x; +(\frac{1}{2}, 0, 0)$ (origin 2)	4*e*	4*j*	4*i*	4*f*	4*g* 2×4*h*	4*h* 8*m*	2*a*;2*b* 2×4*j*	2*c*;2*d* 2×4*i*	8*m* 8*m*	4*k*;4*l* 8*m*	2×4*g* 2×8*m*
[2] *Pncb* (50) ≙ *Pban*	**a**, 2**b**, **c** 2**b**, **c**, **a**	$x, \frac{1}{2}y, z+\frac{1}{4}; +(0, \frac{1}{2}, 0)$ (origin 1) origin 2: $x, \frac{1}{2}y+\frac{1}{4}, z; +(0, \frac{1}{2}, 0)$ $\frac{1}{2}y, z+\frac{1}{4}, x; +(\frac{1}{2}, 0, 0)$ (origin 1) origin 2: $\frac{1}{2}y+\frac{1}{4}, z, x; +(\frac{1}{2}, 0, 0)$	4*i*	4*f*	4*e*	4*j*	2*a*;2*b* 2×4*h*	2*c*;2*d* 2×4*i*	4*g* 8*m*	4*h* 8*m*	4*k*;4*l* 2×4*j*	8*m* 8*m*	2×4*g* 2×8*m*

Wyckoff positions

			2*a*	2*b*	2*c*	2*d*	2*e* 4*l*	2*f* 4*m*	2*g* 4*n*	2*h* 4*o*	4*i* 4*p*	4*j* 4*q*	4*k* 8*r*
Enlarged unit cell, isomorphic													
[2] *Pccm*	2**a**, **b**, **c**	$\frac{1}{2}x, y, z;$ $+(\frac{1}{2}, 0, 0)$	2*a*;2*d*	4*q*	2*b*;2*c*	4*q*	2*e*;2*f* 8*r*	4*i* 4*m*;4*p*	2*g*;2*h* 8*r*	4*j* 4*n*;4*o*	2×4*i* 8*r*	2×4*j* 2×4*q*	4*k*;4*l* 2×8*r*
[2] *Pccm*	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4}, y, z;$ $+(\frac{1}{2}, 0, 0)$	4*q*	2*b*;2*c*	4*q*	2*a*;2*d*	4*i* 4*k*;4*l*	2*e*;2*f* 8*r*	4*j* 4*n*;4*o*	2*g*;2*h* 8*r*	2×4*i* 4*m*;4*p*	2×4*j* 2×4*q*	8*r* 2×8*r*
[3] *Pccm*	3**a**, **b**, **c**	$\frac{1}{3}x, y, z;$ $\pm(\frac{1}{3}, 0, 0)$	2*a*;4*q*	2*b*;4*q*	2*c*;4*q*	2*d*;4*q*	2*e*;4*i* 4*l*;8*r*	2*f*;4*i* 4*m*;8*r*	2*g*;4*j* 4*n*;8*r*	2*h*;4*j* 4*o*;8*r*	3×4*i* 4*p*;8*r*	3×4*j* 3×4*q*	4*k*;8*r* 3×8*r*
[*p*] *Pccm*	*p***a**, **b**, **c**	$\frac{1}{p}x, y, z;$ $+(\frac{u}{p}, 0, 0)$ $p =$ prime > 2; $u = 1, \ldots, p-1$	2*a*; $\frac{p-1}{2}\times 4q$	2*b*; $\frac{p-1}{2}\times 4q$	2*c*; $\frac{p-1}{2}\times 4q$	2*d*; $\frac{p-1}{2}\times 4q$	2*e*; $\frac{p-1}{2}\times 4i$ 4*l*; $\frac{p-1}{2}\times 8r$	2*f*; $\frac{p-1}{2}\times 4i$ 4*m*; $\frac{p-1}{2}\times 8r$	2*g*; $\frac{p-1}{2}\times 4j$ 4*n*; $\frac{p-1}{2}\times 8r$	2*h*; $\frac{p-1}{2}\times 4j$ 4*o*; $\frac{p-1}{2}\times 8r$	$p\times 4i$ 4*p*; $\frac{p-1}{2}\times 8r$	$p\times 4j$ $p\times 4q$	4*k*; $\frac{p-1}{2}\times 8r$ $p\times 8r$
[2] *Pccm*	**a**, 2**b**, **c**	$x, \frac{1}{2}y, z;$ $+(0, \frac{1}{2}, 0)$	2*a*;2*c*	4*q*	4*q*	2*b*;2*d*	2*e*;2*g* 2×4*l*	2*f*;2*h* 4*m*;4*o*	4*k* 8*r*	4*l* 8*r*	4*i*;4*j* 4*n*;4*p*	8*r* 2×4*q*	2×4*k* 2×8*r*
[2] *Pccm*	**a**, 2**b**, **c**	$x, \frac{1}{2}y+\frac{1}{4}, z;$ $+(0, \frac{1}{2}, 0)$	4*q*	2*b*;2*d*	2*a*;2*c*	4*q*	4*k* 2×4*l*	4*l* 8*r*	2*e*;2*g* 4*n*;4*p*	2*f*;2*h* 4*m*;4*o*	8*r* 8*r*	4*i*;4*j* 2×4*q*	2×4*k* 2×8*r*
[3] *Pccm*	**a**,3**b**, **c**	$x, \frac{1}{3}y, z;$ $\pm(0, \frac{1}{3}, 0)$	2*a*;4*q*	2*b*;4*q*	2*c*;4*q*	2*d*;4*q*	2*e*;4*k* 3×4*l*	2*f*;4*l* 4*m*;8*r*	2*g*;4*k* 4*n*;8*r*	2*h*;4*l* 4*o*;8*r*	4*i*;8*r* 4*p*;8*r*	4*j*;8*r* 3×4*q*	3×4*k* 3×8*r*
[*p*] *Pccm*	**a**, *p***b**, **c**	$x, \frac{1}{p}y, z;$ $+(0, \frac{u}{p}, 0)$ $p =$ prime > 2; $u = 1, \ldots, p-1$	2*a*; $\frac{p-1}{2}\times 4q$	2*b*; $\frac{p-1}{2}\times 4q$	2*c*; $\frac{p-1}{2}\times 4q$	2*d*; $\frac{p-1}{2}\times 4q$	2*e*; $\frac{p-1}{2}\times 4k$ $p\times 4l$	2*f*; $\frac{p-1}{2}\times 4l$ 4*m*; $\frac{p-1}{2}\times 8r$	2*g*; $\frac{p-1}{2}\times 4k$ 4*n*; $\frac{p-1}{2}\times 8r$	2*h*; $\frac{p-1}{2}\times 4l$ 4*o*; $\frac{p-1}{2}\times 8r$	4*i*; $\frac{p-1}{2}\times 8r$ 4*p*; $\frac{p-1}{2}\times 8r$	4*j*; $\frac{p-1}{2}\times 8r$ $p\times 4q$	$p\times 4k$ $p\times 8r$

Continued at the bottom of page 513

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Pban No. 50 $P2/b2/a2/n$ D_{2h}^{4}

	Axes	Coordinates origin 1	 origin 2	Wyckoff positions 2*a*	 2*b*	 2*c*	 2*d*	 4*e*	 4*f*	 4*g*	 4*h* 4*k*	 4*i* 4*l*	 4*j* 8*m*
I Maximal *translationengleiche* subgroups													
[2] *Pba*2 (32)			$x+\frac{1}{4},y+\frac{1}{4},z$	2*a*	2*b*	2*b*	2*a*	4*c*	4*c*	4*c*	4*c* 2×2*a*	4*c* 2×2*b*	4*c* 2×4*c*
[2] *P*2*an* (30) ≙ *Pnc*2	 **c**, **b**, −**a**	 $z,y,-x$	$x,y+\frac{1}{4},z$ $z,y+\frac{1}{4},-x$	2*a*	2*a*	2*b*	2*b*	4*c*	4*c*	2×2*a*	2×2*b* 4*c*	4*c* 4*c*	4*c* 2×4*c*
[2] *Pb*2*n* (30) ≙ *Pnc*2	 **c**, **a**, **b**	 z,x,y	$x+\frac{1}{4},y,z$ $z,x+\frac{1}{4},y$	2*a*	2*a*	2*b*	2*b*	4*c*	4*c*	4*c*	4*c* 4*c*	2×2*a* 4*c*	2×2*b* 2×4*c*
[2] *P*222 (16)			$x+\frac{1}{4},y+\frac{1}{4},z$	1*a*; 1*e*	1*b*; 1*c*	1*f*; 1*g*	1*d*; 1*h*	4*u*	4*u*	2*i*; 2*k*	2*j*; 2*l* 2*q*; 2*t*	2*m*; 2*o* 2*r*; 2*s*	2*n*; 2*p* 2×4*u*
[2] $P2/b11$ (13) ≙ $P12/c1$	 **c**, **a**, **b**	$x+\frac{1}{4},y+\frac{1}{4},z$ $z,x+\frac{1}{4},y+\frac{1}{4}$	 z,x,y	2*e*	2*e*	2*f*	2*f*	2*a*; 2*c*	2*b*; 2*d*	2×2*e*	2×2*f* 4*g*	4*g* 4*g*	4*g* 2×4*g*
[2] $P12/a1$ (13) ≙ $P12/c1$	 −**c**, **b**, **a**	$x+\frac{1}{4},y+\frac{1}{4},z$ $-z,y+\frac{1}{4},x+\frac{1}{4}$	 $-z,y,x$	2*e*	2*e*	2*f*	2*f*	2*a*; 2*c*	2*b*; 2*d*	4*g*	4*g* 4*g*	2×2*e* 4*g*	2×2*f* 2×4*g*
[2] $P112/n$ (13)		$x+\frac{1}{4},y+\frac{1}{4},z$		2*e*	2*f*	2*f*	2*e*	2*a*; 2*d*	2*b*; 2*c*	4*g*	4*g* 2×2*e*	4*g* 2×2*f*	4*g* 2×4*g*
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**													
[2] *Pnan* (52) ≙ *Pnna*	**a**, **b**, 2**c** **a**, −2**c**, **b**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z$; $+(0,0,\frac{1}{2})$ $x+\frac{1}{4},-\frac{1}{2}z,y+\frac{1}{4}$; $+(0,\frac{1}{2},0)$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$ $x,-\frac{1}{2}z,y$; $+(0,\frac{1}{2},0)$	4*c*	4*c*	4*d*	4*d*	4*a*; 4*b*	8*e*	8*e*	2×4*d* 8*e*	2×4*c* 8*e*	8*e* 2×8*e*
[2] *Pnan* (52) ≙ *Pnna*	**a**, **b**, 2**c** **a**, −2**c**, **b**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ $x+\frac{1}{4},-\frac{1}{2}z-\frac{1}{4},y+\frac{1}{4}$; $+(0,\frac{1}{2},0)$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ $x,-\frac{1}{2}z-\frac{1}{4},y$; $+(0,\frac{1}{2},0)$	4*d*	4*d*	4*c*	4*c*	8*e*	4*a*; 4*b*	2×4*d*	8*e* 8*e*	8*e* 8*e*	2×4*c* 2×8*e*
[2] *Pbnn* (52) ≙ *Pnna*	**a**, **b**, 2**c** **b**, 2**c**, **a**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z$; $+(0,0,\frac{1}{2})$ $y+\frac{1}{4},\frac{1}{2}z,x+\frac{1}{4}$; $+(0,\frac{1}{2},0)$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$ $y,\frac{1}{2}z,x$; $+(0,\frac{1}{2},0)$	4*c*	4*c*	4*d*	4*d*	4*a*; 4*b*	8*e*	2×4*c*	8*e* 8*e*	8*e* 8*e*	2×4*d* 2×8*e*
[2] *Pbnn* (52) ≙ *Pnna*	**a**, **b**, 2**c** **b**, 2**c**, **a**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ $y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4},x+\frac{1}{4}$; $+(0,\frac{1}{2},0)$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ $y,\frac{1}{2}z+\frac{1}{4},x$; $+(0,\frac{1}{2},0)$	4*d*	4*d*	4*c*	4*c*	8*e*	4*a*; 4*b*	8*e*	2×4*c* 8*e*	2×4*d* 8*e*	8*e* 2×8*e*
[2] *Pnnn* (48)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*k*	4*l*	2*b*; 2*d*	2*a*; 2*c*	4*e*; 4*f*	8*m*	8*m*	4*g*; 4*h* 2×4*k*	8*m* 2×4*l*	4*i*; 4*j* 2×8*m*
[2] *Pnnn* (48)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*a*; 2*c*	2*b*; 2*d*	4*l*	4*k*	8*m*	4*e*; 4*f*	4*g*; 4*h*	8*m* 2×4*k*	4*i*; 4*j* 2×4*l*	8*m* 2×8*m*

Subgroup	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$ $4j$	$4g$ $4k$	$4h$ $4l$	$4i$ $8m$
Enlarged unit cell, isomorphic												
[3] $Pban$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$2a(b^*);4g$	$2b(a^*);4g$	$2c(d^*);4h$	$2d(c^*);4h$	$4e;8m$	$4f;8m$ $4j;8m$	$3\times4g$ $4k(l^*);8m$	$3\times4h$ $4l(k^*);8m$	$4i;8m$ $3\times8m$
[p] $Pban$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$ $p=$ prime >2; $u=1,\dots,p-1$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$	$2a(b^\dagger)$; $\frac{p-1}{2}\times4g$	$2b(a^\dagger)$; $\frac{p-1}{2}\times4g$	$2c(d^\dagger)$; $\frac{p-1}{2}\times4h$	$2d(c^\dagger)$; $\frac{p-1}{2}\times4h$	$4e$; $\frac{p-1}{2}\times8m$	$4f$; $\frac{p-1}{2}\times8m$ $4j$; $\frac{p-1}{2}\times8m$	$p\times4g$ $4k(l^\dagger)$; $\frac{p-1}{2}\times8m$	$p\times4h$ $4l(k^\dagger)$; $\frac{p-1}{2}\times8m$	$4i$; $\frac{p-1}{2}\times8m$ $\frac{p-1}{2}\times8m$
[3] $Pban$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$2a(b^*);4i$	$2b(a^*);4i$	$2c(d^*);4j$	$2d(c^*);4j$	$4e;8m$	$4f;8m$ $3\times4j$	$4g;8m$ $4k(l^*);8m$	$4h;8m$ $4l(k^*);8m$	$3\times4i$ $3\times8m$
[p] $Pban$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$ $p=$ prime >2; $u=1,\dots,p-1$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	$2a(b^\dagger)$; $\frac{p-1}{2}\times4i$	$2b(a^\dagger)$; $\frac{p-1}{2}\times4i$	$2c(d^\dagger)$; $\frac{p-1}{2}\times4j$	$2d(c^\dagger)$; $\frac{p-1}{2}\times4j$	$4e$; $\frac{p-1}{2}\times8m$	$4f$; $\frac{p-1}{2}\times8m$ $p\times4j$	$4g$; $\frac{p-1}{2}\times8m$ $4k(l^\dagger)$; $\frac{p-1}{2}\times8m$	$4h$; $\frac{p-1}{2}\times8m$ $4l(k^\dagger)$; $\frac{p-1}{2}\times8m$	$p\times4i$ $\frac{p-1}{2}\times8m$
[2] $Pban$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a;2d$	$2b;2c$	$4l$	$4k$	$4e;4f$	$8m$ $8m$	$4g;4h$ $2\times4k$	$8m$ $2\times4l$	$4i;4j$ $2\times8m$
[2] $Pban$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4k$	$4l$	$2b;2c$	$2a;2d$	$8m$	$4e;4f$ $4i;4j$	$8m$ $2\times4k$	$4g;4h$ $2\times4l$	$8m$ $2\times8m$
[3] $Pban$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a;4k$	$2b;4l$	$2c;4l$	$2d;4k$	$4e;8m$	$4f;8m$ $4j;8m$	$4g;8m$ $3\times4k$	$4h;8m$ $3\times4l$	$4i;8m$ $3\times8m$
[p] $Pban$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times4k$	$2b$; $\frac{p-1}{2}\times4l$	$2c$; $\frac{p-1}{2}\times4l$	$2d$; $\frac{p-1}{2}\times4k$	$4e$; $\frac{p-1}{2}\times8m$	$4f$; $\frac{p-1}{2}\times8m$ $4j$; $\frac{p-1}{2}\times8m$	$4g$; $\frac{p-1}{2}\times8m$ $p\times4k$	$4h$; $\frac{p-1}{2}\times8m$ $p\times4l$	$4i$; $\frac{p-1}{2}\times8m$ $\frac{p-1}{2}\times8m$

* origin 2 $\quad$ † origin 2 and $p=4n-1$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pncb$ $\quad a\to b\to c\to a \quad \mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a} \quad x\to y\to z\to x$

$Pcna$ $\quad a\leftarrow b\leftarrow c\leftarrow a \quad \mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a} \quad x\leftarrow y\leftarrow z\leftarrow x$

Pmma No. 51 $P2_1/m2/m2/a$ D_{2h}^5

	Axes	Coordinates	Wyckoff positions 2*a*	 2*b*	 2*c*	 2*d*	 2*e*	 2*f*	 4*g*	 4*h*	 4*i* 4*k*	 4*j* 8*l*
I Maximal *translationengleiche* subgroups												
[2] *Pm*2*a* (28) ≙ *Pma*2	**a**, **c**, −**b**	$x,z,-y$	2*a*	2*a*	2*b*	2*b*	2*c*	2*c*	2×2*a*	2×2*b*	4*d* 2×2*c*	4*d* 2×4*d*
[2] $P2_1ma$ (26) ≙ $Pmc2_1$	**b**, **c**, **a**	y,z,x	2*a*	2*b*	2*a*	2*b*	2*a*	2*b*	4*c*	4*c*	2×2*a* 4*c*	2×2*b* 2×4*c*
[2] *Pmm*2 (25)		$x+\frac{1}{4},y,z$	2*e*	2*f*	2*e*	2*f*	1*a*; 1*c*	1*b*; 1*d*	4*i*	4*i*	2×2*e* 2*g*; 2*h*	2×2*f* 2×4*i*
[2] $P2_122$ (17) ≙ $P222_1$	**b**, **c**, **a**	y,z,x	2*a*	2*a*	2*b*	2*b*	2*c*	2*d*	2×2*a*	2×2*b*	4*e* 4*e*	4*e* 2×4*e*
[2] $P112/a$ (13) ≙ $P12/c1$	**b**, **c**, **a**	y,z,x	2*a*	2*d*	2*c*	2*b*	2*e*	2*f*	4*g*	4*g*	4*g* 4*g*	4*g* 2×4*g*
[2] $P2_1/m11$ (11) ≙ $P12_1/m1$	**c**, **a**, **b**	z,x,y	2*a*	2*c*	2*b*	2*d*	2*e*	2*e*	4*f*	4*f*	4*f* 2×2*e*	4*f* 2×4*f*
[2] $P12/m1$ (10)			1*a*; 1*d*	1*b*; 1*e*	1*c*; 1*g*	1*f*; 1*h*	2*m*	2*n*	2*i*; 2*j*	2*k*; 2*l*	2×2*m* 4*o*	2×2*n* 2×4*o*
II Maximal *klassengleiche* subgroups												
Enlarged unit cell, non-isomorphic *see next page*												
Enlarged unit cell, isomorphic												
[3] *Pmma*	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;$ $\pm(\frac{1}{3},0,0)$	2*a*; 4*i*	2*b*; 4*j*	2*c*; 4*i*	2*d*; 4*j*	2*e*; 4*i*	2*f*; 4*j*	4*g*; 8*l*	4*h*; 8*l*	3×4*i* 4*k*; 8*l*	3×4*j* 3×8*l*
[*p*] *Pmma* p = prime > 2; $u = 1,\ldots,p-1$	*p***a**, **b**, **c**	$\frac{1}{p}x,y,z;$ $+(\frac{u}{p},0,0)$	2*a*; $\frac{p-1}{2}\times 4i$	2*b*; $\frac{p-1}{2}\times 4j$	2*c*; $\frac{p-1}{2}\times 4i$	2*d*; $\frac{p-1}{2}\times 4j$	2*e*; $\frac{p-1}{2}\times 4i$	2*f*; $\frac{p-1}{2}\times 4j$	4*g*; $\frac{p-1}{2}\times 8l$	4*h*; $\frac{p-1}{2}\times 8l$	$p\times 4i$ 4*k*; $\frac{p-1}{2}\times 8l$	$p\times 4j$ $p\times 8l$
[2] *Pmma*	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;$ $+(0,\frac{1}{2},0)$	2*a*; 2*b*	4*g*	2*c*; 2*d*	4*h*	2*e*; 2*f*	4*k*	2×4*g*	2×4*h*	4*i*; 4*j* 2×4*k*	8*l* 2×8*l*
[2] *Pmma*	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;$ $+(0,\frac{1}{2},0)$	4*g*	2*a*; 2*b*	4*h*	2*c*; 2*d*	4*k*	2*e*; 2*f*	2×4*g*	2×4*h*	8*l* 2×4*k*	4*i*; 4*j* 2×8*l*
[3] *Pmma*	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;$ $\pm(0,\frac{1}{3},0)$	2*a*; 4*g*	2*b*; 4*g*	2*c*; 4*h*	2*d*; 4*h*	2*e*; 4*k*	2*f*; 4*k*	3×4*g*	3×4*h*	4*i*; 8*l* 3×4*k*	4*j*; 8*l* 3×8*l*
[*p*] *Pmma* p = prime > 2; $u = 1,\ldots,p-1$	**a**, *p***b**, **c**	$x,\frac{1}{p}y,z;$ $+(0,\frac{u}{p},0)$	2*a*; $\frac{p-1}{2}\times 4g$	2*b*; $\frac{p-1}{2}\times 4g$	2*c*; $\frac{p-1}{2}\times 4h$	2*d*; $\frac{p-1}{2}\times 4h$	2*e*; $\frac{p-1}{2}\times 4k$	2*f*; $\frac{p-1}{2}\times 4k$	$p\times 4g$	$p\times 4h$	4*i*; $\frac{p-1}{2}\times 8l$ $p\times 4k$	4*j*; $\frac{p-1}{2}\times 8l$ $p\times 8l$
[2] *Pmma*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	2*a*; 2*c*	2*b*; 2*d*	4*i*	4*j*	2×2*e*	2×2*f*	4*g*; 4*h*	8*l*	2×4*i* 2×4*k*	2×4*j* 2×8*l*
[2] *Pmma*	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	4*i*	4*j*	2*a*; 2*c*	2*b*; 2*d*	2×2*e*	2×2*f*	8*l*	4*g*; 4*h*	2×4*i* 2×4*k*	2×4*j* 2×8*l*
[3] *Pmma*	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	2*a*; 4*i*	2*b*; 4*j*	2*c*; 4*i*	2*d*; 4*j*	3×2*e*	3×2*f*	4*g*; 8*l*	4*h*; 8*l*	3×4*i* 3×4*k*	3×4*j* 3×8*l*
[*p*] *Pmma* p = prime > 2; $u = 1,\ldots,p-1$	**a**, **b**, *p***c**	$x,y,\frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	2*a*; $\frac{p-1}{2}\times 4i$	2*b*; $\frac{p-1}{2}\times 4j$	2*c*; $\frac{p-1}{2}\times 4i$	2*d*; $\frac{p-1}{2}\times 4j$	$p\times 2e$	$p\times 2f$	4*g*; $\frac{p-1}{2}\times 8l$	4*h*; $\frac{p-1}{2}\times 8l$	$p\times 4i$ $p\times 4k$	$p\times 4j$ $p\times 8l$

	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$	$2e$	$2f$	$4g$	$4h$	$4i$ $4k$	$4j$ $8l$
Enlarged unit cell, non-isomorphic												
[2] *Aema* (64) ≙*Cmce*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y, \frac{1}{2}z, x; +(\frac{1}{2},0,0)$	$4a;4b$	$8d$	$8f$	$8c$	$8f$	$8e$	$2\times8d$	$16g$	$2\times8f$ $16g$	$16g$ $2\times16g$
[2] *Aema* (64) ≙*Cmce*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z, x; +(\frac{1}{2},0,0)$	$8d$	$4a;4b$	$8c$	$8f$	$8e$	$8f$	$2\times8d$	$16g$	$16g$ $16g$	$2\times8f$ $2\times16g$
[2] *Aema* (64) ≙*Cmce*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}; +(0,\frac{1}{2},0)$ $\frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2},0,0)$	$8f$	$8c$	$4a;4b$	$8d$	$8f$	$8e$	$16g$	$2\times8d$	$2\times8f$ $16g$	$16g$ $2\times16g$
[2] *Aema* (64) ≙*Cmce*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(0,\frac{1}{2},0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2},0,0)$	$8c$	$8f$	$8d$	$4a;4b$	$8e$	$8f$	$16g$	$2\times8d$	$16g$ $16g$	$2\times8f$ $2\times16g$
[2] *Amma* (63) ≙*Cmcm*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y, \frac{1}{2}z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y, \frac{1}{2}z, x; +(\frac{1}{2},0,0)$	$4a;4b$	$8e$	$8f$	$8d$	$2\times4c$	$8g$	$2\times8e$	$16h$	$2\times8f$ $2\times8g$	$16h$ $2\times16h$
[2] *Amma* (63) ≙*Cmcm*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z, x; +(\frac{1}{2},0,0)$	$8e$	$4a;4b$	$8d$	$8f$	$8g$	$2\times4c$	$2\times8e$	$16h$	$16h$ $2\times8g$	$2\times8f$ $2\times16h$
[2] *Amma* (63) ≙*Cmcm*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}; +(0,\frac{1}{2},0)$ $\frac{1}{2}y, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2},0,0)$	$8f$	$8d$	$4a;4b$	$8e$	$2\times4c$	$8g$	$16h$	$2\times8e$	$2\times8f$ $2\times8g$	$16h$ $2\times16h$
[2] *Amma* (63) ≙*Cmcm*	**a**, 2**b**, 2**c** 2**b**, 2**c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(0,\frac{1}{2},0)$ $\frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}, x; +(\frac{1}{2},0,0)$	$8d$	$8f$	$8e$	$4a;4b$	$8g$	$2\times4c$	$16h$	$2\times8e$	$16h$ $2\times8g$	$2\times8f$ $2\times16h$
[2] *Pmmn* (59)	**a**, 2**b**, **c**	origin 1: $x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$ origin 2: $x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$	$4c$	$4f$	$4d$	$4f$	$4e$	$2a;2b$	$8g$	$8g$	$8g$ $2\times4e$	$2\times4f$ $2\times8g$
[2] *Pmmn* (59)	**a**, 2**b**, **c**	origin 1: $x+\frac{1}{4}, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$ origin 2: $x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$	$4f$	$4c$	$4f$	$4d$	$2a;2b$	$4e$	$8g$	$8g$	$2\times4f$ $2\times4e$	$8g$ $2\times8g$
[2] *Pbma* (57) ≙*Pbcm*	**a**, 2**b**, **c** **c**, **a**, 2**b**	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$ $z, x, \frac{1}{2}y; +(0,0,\frac{1}{2})$	$4a$	$4d$	$4b$	$4d$	$4c$	$4d$	$8e$	$8e$	$8e$ $8e$	$2\times4d$ $2\times8e$
[2] *Pbma* (57) ≙*Pbcm*	**a**, 2**b**, **c** **c**, **a**, 2**b**	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$ $z, x, \frac{1}{2}y+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4d$	$4a$	$4d$	$4b$	$4d$	$4c$	$8e$	$8e$	$2\times4d$ $8e$	$8e$ $2\times8e$
[2] *Pmca* (57) ≙*Pbcm*	**a**, **b**, 2**c** **b**, 2**c**, **a**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$ $y, \frac{1}{2}z, x; +(0,\frac{1}{2},0)$	$4a$	$4b$	$4c$	$4c$	$4d$	$4d$	$8e$	$2\times4c$	$8e$ $2\times4d$	$8e$ $2\times8e$
[2] *Pmca* (57) ≙*Pbcm*	**a**, **b**, 2**c** **b**, 2**c**, **a**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$ $y, \frac{1}{2}z+\frac{1}{4}, x; +(0,\frac{1}{2},0)$	$4c$	$4c$	$4a$	$4b$	$4d$	$4d$	$2\times4c$	$8e$	$8e$ $2\times4d$	$8e$ $2\times8e$
[2] *Pcma* (55) ≙*Pbam*	**a**, **b**, 2**c** 2**c**, **a**, **b**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$ $\frac{1}{2}z, x, y; +(\frac{1}{2},0,0)$	$2a;2c$	$2b;2d$	$4g$	$4h$	$4g$	$4h$	$4e;4f$	$8i$	$2\times4g$ $8i$	$2\times4h$ $2\times8i$
[2] *Pcma* (55) ≙*Pbam*	**a**, **b**, 2**c** 2**c**, **a**, **b**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$ $\frac{1}{2}z+\frac{1}{4}, x, y; +(\frac{1}{2},0,0)$	$4g$	$4h$	$2a;2c$	$2b;2d$	$4g$	$4h$	$8i$	$4e;4f$	$2\times4g$ $8i$	$2\times4h$ $2\times8i$
[2] *Pcca* (54)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$4a$	$4b$	$4c$	$4c$	$4d$	$4e$	$8f$	$2\times4c$	$8f$ $8f$	$8f$ $2\times8f$
[2] *Pcca* (54)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4c$	$4c$	$4a$	$4b$	$4d$	$4e$	$2\times4c$	$8f$	$8f$ $8f$	$8f$ $2\times8f$
[2] *Pbmn* (53) ≙*Pmna*	**a**, 2**b**, **c** 2**b**, **c**, **a**	$x, \frac{1}{2}y, z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y, z, x; +(\frac{1}{2},0,0)$	$2a;2b$	$4e$	$2c;2d$	$4f$	$4h$	$4g$	$2\times4e$	$2\times4f$	$2\times4h$ $8i$	$8i$ $2\times8i$
[2] *Pbmn* (53) ≙*Pmna*	**a**, 2**b**, **c** 2**b**, **c**, **a**	$x, \frac{1}{2}y+\frac{1}{4}, z; +(0,\frac{1}{2},0)$ $\frac{1}{2}y+\frac{1}{4}, z, x; +(\frac{1}{2},0,0)$	$4e$	$2a;2b$	$4f$	$2c;2d$	$4g$	$4h$	$2\times4e$	$2\times4f$	$8i$ $8i$	$2\times4h$ $2\times8i$

Continued at the bottom of the next page

Pnna No. 52 $P2/n2_1/n2/a$ D_{2h}^6

	Axes	Coordinates	Wyckoff positions 4*a*	4*b*	4*c*	4*d*	8*e*
I Maximal *translationengleiche* subgroups							
[2] *Pnn*2 (34)		$x+\frac{1}{4},y,z$	4*c*	4*c*	2*a*; 2*b*	4*c*	2×4*c*
[2] $Pn2_1a$ (33)		$x+\frac{1}{4},y,z+\frac{1}{4}$	4*a*	4*a*	4*a*	4*a*	2×4*a*
$\widehat{=}$ $Pna2_1$	**a**, **c**, −**b**	$x+\frac{1}{4},z+\frac{1}{4},-y$					
[2] *P*2*na* (30)		$x,y+\frac{1}{4},z+\frac{1}{4}$	4*c*	4*c*	4*c*	2*a*; 2*b*	2×4*c*
$\widehat{=}$ *Pnc*2	**b**, **c**, **a**	$y+\frac{1}{4},z+\frac{1}{4},x$					
[2] $P22_12$ (17)		$x+\frac{1}{4},y,z+\frac{1}{4}$	4*e*	4*e*	2*a*; 2*b*	2*c*; 2*d*	2×4*e*
$\widehat{=}$ $P222_1$	**c**, **a**, **b**	$z+\frac{1}{4},x+\frac{1}{4},y$					
[2] $P12_1/n1$ (14)			2*a*; 2*d*	2*b*; 2*c*	4*e*	4*e*	2×4*e*
[2] $P2/n11$ (13)			2*a*; 2*c*	2*b*; 2*d*	4*g*	2*e*; 2*f*	2×4*g*
$\widehat{=}$ $P12/n1$	**c**, **a**, **b**	z,x,y					
[2] $P112/a$ (13)			2*a*; 2*b*	2*c*; 2*d*	2*e*; 2*f*	4*g*	2×4*g*
$\widehat{=}$ $P12/c1$	**b**, **c**, **a**	y,z,x					
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[3] *Pnna*	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	4*a*; 8*e*	4*b*; 8*e*	4*c*; 8*e*	3×4*d*	3×8*e*
[*p*] *Pnna*	*p***a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	4*a*; $\frac{p-1}{2}$×8*e*	4*b*; $\frac{p-1}{2}$×8*e*	4*c*; $\frac{p-1}{2}$×8*e*	*p*×4*d*	*p*×8*e*
	p = prime > 2; $u = 1,\ldots,p-1$						
[3] *Pnna*	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	4*a*; 8*e*	4*b*; 8*e*	4*c*; 8*e*	4*d*; 8*e*	3×8*e*
[*p*] *Pnna*	**a**, *p***b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	4*a*; $\frac{p-1}{2}$×8*e*	4*b*; $\frac{p-1}{2}$×8*e*	4*c*; $\frac{p-1}{2}$×8*e*	4*d*; $\frac{p-1}{2}$×8*e*	*p*×8*e*
	p = prime > 2; $u = 1,\ldots,p-1$						
[3] *Pnna*	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	4*a*; 8*e*	4*b*; 8*e*	3×4*c*	4*d*; 8*e*	3×8*e*
[*p*] *Pnna*	**a**, **b**, *p***c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	4*a*; $\frac{p-1}{2}$×8*e*	4*b*; $\frac{p-1}{2}$×8*e*	*p*×4*c*	4*d*; $\frac{p-1}{2}$×8*e*	*p*×8*e*
	p = prime > 2; $u = 1,\ldots,p-1$						

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Pbnn	$a \rightarrow b;\ c \rightarrow a$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
Pncn	$a \rightarrow c;\ c \rightarrow b$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
Pnnb	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
Pcnn	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
Pnan	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

Pmma No. 51 $P2_1/m2/m2/a$ CONTINUED *(from preceding page)*

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Pbmm	$A \rightarrow B;\ C \rightarrow A$	$a \rightarrow b \rightarrow c \rightarrow a$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
Pmcm	$A \rightarrow C;\ C \rightarrow B$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
Pmmb	$A \rightarrow B$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
Pcmm	$A \rightleftarrows C$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
Pmam	$C \rightarrow B$	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

D_{2h}^{7} $P2/m2/n2_1/a$ No. 53 $Pmna$

	Axes	Coordinates	Wyckoff positions 2a	2b	2c	2d	4e	4f	4g	4h	8i
I Maximal *translationengleiche* subgroups											
[2] $Pmn2_1$ (31)			2a	2a	2a	2a	4b	4b	4b	2×2a	2×4b
[2] $P2na$ (30)			2a	2a	2b	2b	2×2a	2×2b	4c	4c	2×4c
≙ $Pnc2$	**b**, **c**, **a**	y,z,x									
[2] $Pm2a$ (28)		$x+\frac{1}{4},y,z+\frac{1}{4}$	2c	2c	2c	2c	4d	4d	2a; 2b	2×2c	2×4d
≙ $Pma2$	**a**, **c**, −**b**	$x+\frac{1}{4},z+\frac{1}{4},-y$									
[2] $P222_1$ (17)		$x+\frac{1}{4},y,z$	2a	2a	2b	2b	2×2a	2×2b	2c; 2d	4e	2×4e
[2] $P112_1/a$ (14)			2a	2c	2d	2b	4e	4e	4e	4e	2×4e
[2] $P12/n1$ (13)			2a	2d	2b	2c	4g	4g	2e; 2f	4g	2×4g
[2] $P2/m11$ (10)			1a; 1e	1b; 1d	1f; 1g	1c; 1h	2i; 2j	2k; 2l	4o	2m; 2n	2×4o
≙ $P12/m1$	**c**, **a**, **b**	z,x,y									
II Maximal *klassengleiche* subgroups											
Enlarged unit cell, non-isomorphic											
[2] $Pbna$ (60)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	4a	4b	4c	4c	8d	2×4c	8d	8d	2×8d
≙ $Pbcn$	**c**, **a**, 2**b**	$z,x,\frac{1}{2}y;\ +(0,0,\frac{1}{2})$									
[2] $Pbna$ (60)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	4c	4c	4b	4a	2×4c	8d	8d	8d	2×8d
≙ $Pbcn$	**c**, **a**, 2**b**	$z,x,\frac{1}{2}y+\frac{1}{4};\ +(0,0,\frac{1}{2})$									
[2] $Pmnn$ (58)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2a; 2d	2b; 2c	4g	4g	4e; 4f	8h	8h	2×4g	2×8h
≙ $Pnnm$	2**b**, **c**, **a**	$\frac{1}{2}y,z,x;\ +(\frac{1}{2},0,0)$									
[2] $Pmnn$ (58)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	4g	4g	2b; 2c	2a; 2d	8h	4e; 4f	8h	2×4g	2×8h
≙ $Pnnm$	2**b**, **c**, **a**	$\frac{1}{2}y+\frac{1}{4},z,x;\ +(\frac{1}{2},0,0)$									
[2] $Pbnn$ (52)	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	4a	4b	4c	4c	8e	2×4c	2×4d	8e	2×8e
≙ $Pnna$	2**b**, **c**, **a**	$\frac{1}{2}y,z,x;\ +(\frac{1}{2},0,0)$									
[2] $Pbnn$ (52)	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	4c	4c	4b	4a	2×4c	8e	2×4d	8e	2×8e
≙ $Pnna$	2**b**, **c**, **a**	$\frac{1}{2}y+\frac{1}{4},z,x;\ +(\frac{1}{2},0,0)$									
Enlarged unit cell, isomorphic											
[3] $Pmna$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	2a; 4e	2b; 4e	2c; 4f	2d; 4f	3×4e	3×4f	4g; 8i	4h; 8i	3×8i
[p] $Pmna$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$ p = prime > 2; $u=1,\dots,p-1$	2a; $\frac{p-1}{2}$×4e	2b; $\frac{p-1}{2}$×4e	2c; $\frac{p-1}{2}$×4f	2d; $\frac{p-1}{2}$×4f	p×4e	p×4f	4g; $\frac{p-1}{2}$×8i	4h; $\frac{p-1}{2}$×8i	p×8i
[2] $Pmna$	**a**, 2**b**, **c**	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	2a; 2d	2b; 2c	4h	4h	4e; 4f	8i	2×4g	2×4h	2×8i
[2] $Pmna$	**a**, 2**b**, **c**	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	4h	4h	2b; 2c	2a; 2d	8i	4e; 4f	2×4g	2×4h	2×8i
[3] $Pmna$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	2a; 4h	2b; 4h	2c; 4h	2d; 4h	4e; 8i	4f; 8i	3×4g	3×4h	3×8i
[p] $Pmna$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$ p = prime > 2; $u=1,\dots,p-1$	2a; $\frac{p-1}{2}$×4h	2b; $\frac{p-1}{2}$×4h	2c; $\frac{p-1}{2}$×4h	2d; $\frac{p-1}{2}$×4h	4e; $\frac{p-1}{2}$×8i	4f; $\frac{p-1}{2}$×8i	p×4g	p×4h	p×8i
[3] $Pmna$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	2a; 4h	2b; 4h	2c; 4h	2d; 4h	4e; 8i	4f; 8i	4g; 8i	3×4h	3×8i
[p] $Pmna$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime > 2; $u=1,\dots,p-1$	2a; $\frac{p-1}{2}$×4h	2b; $\frac{p-1}{2}$×4h	2c; $\frac{p-1}{2}$×4h	2d; $\frac{p-1}{2}$×4h	4e; $\frac{p-1}{2}$×8i	4f; $\frac{p-1}{2}$×8i	4g; $\frac{p-1}{2}$×8i	p×4h	p×8i

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pbmn$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Pncm$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
$Pnmb$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
$Pcnm$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
$Pman$	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

$Pcca$ No. 54 $P2_1/c2/c2/a$ D_{2h}^8

	Axes	Coordinates	4a	4b	4c	4d	4e	8f
I Maximal *translationengleiche* subgroups								
[2] $Pc2a$ (32)		$x,y,z+\frac{1}{4}$	$4c$	$4c$	$2a;2b$	$4c$	$4c$	$2\times4c$
$\widehat{=}$ $Pba2$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$z+\frac{1}{4},x,y$						
[2] $P2_1ca$ (29)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4a$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $Pca2_1$	$\mathbf{c},-\mathbf{b},\mathbf{a}$	$z+\frac{1}{4},-y,x$						
[2] $Pcc2$ (27)		$x+\frac{1}{4},y,z$	$4e$	$4e$	$4e$	$2a;2c$	$2b;2d$	$2\times4e$
[2] $P2_122$ (17)		$x,y,z+\frac{1}{4}$	$4e$	$4e$	$2a;2b$	$2\times2c$	$2\times2d$	$2\times4e$
$\widehat{=}$ $P222_1$	$\mathbf{b},\mathbf{c},\mathbf{a}$	$y,z+\frac{1}{4},x$						
[2] $P2_1/c11$ (14)			$2a;\ 2c$	$2b;\ 2d$	$4e$	$4e$	$4e$	$2\times4e$
$\widehat{=}$ $P12_1/c1$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y,-x,z$						
[2] $P12/c1$ (13)			$2a;\ 2d$	$2b;\ 2c$	$2e;\ 2f$	$4g$	$4g$	$2\times4g$
[2] $P112/a$ (13)			$2a;\ 2c$	$2b;\ 2d$	$4g$	$2\times2e$	$2\times2f$	$2\times4g$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $Pnca$ (60)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$4a;\ 4b$	$8d$	$8d$	$2\times4c$	$8d$	$2\times8d$
$\widehat{=}$ $Pbcn$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	$\frac{1}{2}y,z,x;\ +(\frac{1}{2},0,0)$						
[2] $Pnca$ (60)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$8d$	$4a;\ 4b$	$8d$	$8d$	$2\times4c$	$2\times8d$
$\widehat{=}$ $Pbcn$	$2\mathbf{b},\mathbf{c},\mathbf{a}$	$\frac{1}{2}y+\frac{1}{4},z,x;\ +(\frac{1}{2},0,0)$						
[2] $Pccn$ (56)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$4a;\ 4b$	$8e$	$8e$	$8e$	$4c;\ 4d$	$2\times8e$
[2] $Pccn$ (56)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$8e$	$4a;\ 4b$	$8e$	$4c;\ 4d$	$8e$	$2\times8e$
[2] $Pncn$ (52)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$4a;\ 4b$	$8e$	$2\times4c$	$8e$	$2\times4d$	$2\times8e$
$\widehat{=}$ $Pnna$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	$z,x,\frac{1}{2}y;\ +(0,0,\frac{1}{2})$						
[2] $Pncn$ (52)	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$8e$	$4a;\ 4b$	$2\times4c$	$2\times4d$	$8e$	$2\times8e$
$\widehat{=}$ $Pnna$	$\mathbf{c},\mathbf{a},2\mathbf{b}$	$z,x,\frac{1}{2}y+\frac{1}{4};\ +(0,0,\frac{1}{2})$						
Enlarged unit cell, isomorphic								
[3] $Pcca$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4c;\ 8f$	$4d;\ 8f$	$4e;\ 8f$	$3\times8f$
[p] $Pcca$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8f$	$4c;\frac{p-1}{2}\times8f$	$4d;\frac{p-1}{2}\times8f$	$4e;\frac{p-1}{2}\times8f$	$p\times8f$
	$p=$ prime $>2;\ u=1,\ldots,p-1$							
[2] $Pcca$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y,z;\ +(0,\frac{1}{2},0)$	$4a;\ 4b$	$8f$	$2\times4c$	$4d;\ 4e$	$8f$	$2\times8f$
[2] $Pcca$	$\mathbf{a},2\mathbf{b},\mathbf{c}$	$x,\frac{1}{2}y+\frac{1}{4},z;\ +(0,\frac{1}{2},0)$	$8f$	$4a;\ 4b$	$2\times4c$	$8f$	$4d;\ 4e$	$2\times8f$
[3] $Pcca$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;\ 8f$	$4b;\ 8f$	$3\times4c$	$4d;\ 8f$	$4e;\ 8f$	$3\times8f$
[p] $Pcca$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8f$	$p\times4c$	$4d;\frac{p-1}{2}\times8f$	$4e;\frac{p-1}{2}\times8f$	$p\times8f$
	$p=$ prime $>2;\ u=1,\ldots,p-1$							
[3] $Pcca$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$4a;\ 8f$	$4b;\ 8f$	$4c;\ 8f$	$3\times4d$	$3\times4e$	$3\times8f$
[p] $Pcca$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8f$	$4c;\frac{p-1}{2}\times8f$	$p\times4d$	$p\times4e$	$p\times8f$
	$p=$ prime $>2;\ u=1,\ldots,p-1$							

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pbaa$	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
$Pbcb$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$
$Pccb$	$a\rightleftarrows b$	$\mathbf{a}\rightleftarrows-\mathbf{b}$	$x\rightleftarrows-y$
$Pcaa$	$a\rightleftarrows c$	$\mathbf{a}\rightleftarrows-\mathbf{c}$	$x\rightleftarrows-z$
$Pbab$	$b\rightleftarrows c$	$\mathbf{b}\rightleftarrows-\mathbf{c}$	$y\rightleftarrows-z$

D_{2h}^{9} $\quad P2_1/b2_1/a2/m$ $\quad$ No. 55 $\quad$ $Pbam$

	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$8i$
I Maximal *translationengleiche* subgroups											
[2] $Pba2$ (32)			$2a$	$2a$	$2b$	$2b$	$2\times2a$	$2\times2b$	$4c$	$4c$	$2\times4c$
[2] $Pb2_1m$ (26)		$x+\frac{1}{4},y,z$	$2a$	$2b$	$2a$	$2b$	$4c$	$4c$	$2\times2a$	$2\times2b$	$2\times4c$
$\widehat{=}$ $Pmc2_1$	**c**, **a**, **b**	$z,x+\frac{1}{4},y$									
[2] $P2_1am$ (26)		$x,y+\frac{1}{4},z$	$2a$	$2b$	$2a$	$2b$	$4c$	$4c$	$2\times2a$	$2\times2b$	$2\times4c$
$\widehat{=}$ $Pmc2_1$	**c**, **b**, −**a**	$z,y+\frac{1}{4},-x$									
[2] $P2_12_12$ (18)			$2a$	$2a$	$2b$	$2b$	$2\times2a$	$2\times2b$	$4c$	$4c$	$2\times4c$
[2] $P2_1/b11$ (14)			$2a$	$2b$	$2c$	$2d$	$4e$	$4e$	$4e$	$4e$	$2\times4e$
$\widehat{=}$ $P12_1/c1$	**c**, **a**, **b**	z,x,y									
[2] $P12_1/a1$ (14)			$2a$	$2d$	$2c$	$2b$	$4e$	$4e$	$4e$	$4e$	$2\times4e$
[2] $P112/m$ (10)			$1a;1g$	$1b;1h$	$1c;1d$	$1e;1f$	$2i;2l$	$2j;2k$	$2\times2m$	$2\times2n$	$2\times4o$
II Maximal *klassengleiche* subgroups											
Enlarged unit cell, non-isomorphic											
[2] $Pnam$ (62)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4c$	$4b$	$4c$	$8d$	$8d$	$8d$	$2\times4c$	$2\times8d$
$\widehat{=}$ $Pnma$	**a**, 2**c**, −**b**	$x,\frac{1}{2}z,-y;\ +(0,\frac{1}{2},0)$									
[2] $Pnam$ (62)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4c$	$4a$	$4c$	$4b$	$8d$	$8d$	$2\times4c$	$8d$	$2\times8d$
$\widehat{=}$ $Pnma$	**a**, 2**c**, −**b**	$x,\frac{1}{2}z+\frac{1}{4},-y;+(0,\frac{1}{2},0)$									
[2] $Pbnm$ (62)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4c$	$4b$	$4c$	$8d$	$8d$	$8d$	$2\times4c$	$2\times8d$
$\widehat{=}$ $Pnma$	**b**, 2**c**, **a**	$y,\frac{1}{2}z,x;\ +(0,\frac{1}{2},0)$									
[2] $Pbnm$ (62)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4c$	$4a$	$4c$	$4b$	$8d$	$8d$	$2\times4c$	$8d$	$2\times8d$
$\widehat{=}$ $Pnma$	**b**, 2**c**, **a**	$y,\frac{1}{2}z+\frac{1}{4},x;\ +(0,\frac{1}{2},0)$									
[2] $Pnnm$ (58)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a;2b$	$4e$	$2c;2d$	$4f$	$2\times4e$	$2\times4f$	$2\times4g$	$8h$	$2\times8h$
[2] $Pnnm$ (58)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4e$	$2a;2b$	$4f$	$2c;2d$	$2\times4e$	$2\times4f$	$8h$	$2\times4g$	$2\times8h$
Enlarged unit cell, isomorphic											
[3] $Pbam$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$2a;4g$	$2b;4h$	$2c;4g$	$2d;4h$	$4e;8i$	$4f;8i$	$3\times4g$	$3\times4h$	$3\times8i$
[p] $Pbam$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$ $p=$ prime >2; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}\times4g$	$2b;$ $\frac{p-1}{2}\times4h$	$2c;$ $\frac{p-1}{2}\times4g$	$2d;$ $\frac{p-1}{2}\times4h$	$4e;$ $\frac{p-1}{2}\times8i$	$4f;$ $\frac{p-1}{2}\times8i$	$p\times4g$	$p\times4h$	$p\times8i$
[3] $Pbam$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$2a;4g$	$2b;4h$	$2c;4g$	$2d;4h$	$4e;8i$	$4f;8i$	$3\times4g$	$3\times4h$	$3\times8i$
[p] $Pbam$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$ $p=$ prime >2; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}\times4g$	$2b;$ $\frac{p-1}{2}\times4h$	$2c;$ $\frac{p-1}{2}\times4g$	$2d;$ $\frac{p-1}{2}\times4h$	$4e;$ $\frac{p-1}{2}\times8i$	$4f;$ $\frac{p-1}{2}\times8i$	$p\times4g$	$p\times4h$	$p\times8i$
[2] $Pbam$	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a;2b$	$4e$	$2c;2d$	$4f$	$2\times4e$	$2\times4f$	$4g;4h$	$8i$	$2\times8i$
[2] $Pbam$	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4e$	$2a;2b$	$4f$	$2c;2d$	$2\times4e$	$2\times4f$	$8i$	$4g;4h$	$2\times8i$
[3] $Pbam$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$2c;4f$	$2d;4f$	$3\times4e$	$3\times4f$	$4g;8i$	$4h;8i$	$3\times8i$
[p] $Pbam$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}\times4e$	$2b;$ $\frac{p-1}{2}\times4e$	$2c;$ $\frac{p-1}{2}\times4f$	$2d;$ $\frac{p-1}{2}\times4f$	$p\times4e$	$p\times4f$	$4g;$ $\frac{p-1}{2}\times8i$	$4h;$ $\frac{p-1}{2}\times8i$	$p\times8i$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pmcb$	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
$Pcma$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

$Pccn$ No. 56 $P2_1/c2_1/c2/n$ D_{2h}^{10}

	Axes	Coordinates	Wyckoff positions $4a$	$4b$	$4c$	$4d$	$8e$
I Maximal *translationengleiche* subgroups							
[2] $P2_1cn$ (33)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $Pna2_1$	$\mathbf{c},\mathbf{b},-\mathbf{a}$	$z+\frac{1}{4},y,-x$					
[2] $Pc2_1n$ (33)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $Pna2_1$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$z+\frac{1}{4},x,y$					
[2] $Pcc2$ (27)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4e$	$4e$	$2a$; $2d$	$2b$; $2c$	$2\times4e$
[2] $P2_12_12$ (18)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$2\times2a$	$2\times2b$	$2\times4c$
[2] $P2_1/c11$ (14)			$2a$; $2d$	$2b$; $2c$	$4e$	$4e$	$2\times4e$
$\widehat{=}$ $P12_1/c1$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y,-x,z$					
[2] $P12_1/c1$ (14)			$2a$; $2d$	$2b$; $2c$	$4e$	$4e$	$2\times4e$
[2] $P112/n$ (13)			$2a$; $2b$	$2c$; $2d$	$2\times2e$	$2\times2f$	$2\times4g$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[3] $Pccn$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$4a$; $8e$	$4b$; $8e$	$4d$; $8e$	$4c$; $8e$	$3\times8e$
[p] $Pccn$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$	$4a$; $\frac{p-1}{2}\times8e$	$4b$; $\frac{p-1}{2}\times8e$	$4c(d^*)$; $\frac{p-1}{2}\times8e$	$4d(c^*)$; $\frac{p-1}{2}\times8e$	$p\times8e$
	p = prime >2; $u=1,\ldots,p-1$						
[3] $Pccn$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$4a$; $8e$	$4b$; $8e$	$4d$; $8e$	$4c$; $8e$	$3\times8e$
[p] $Pccn$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	$4a$; $\frac{p-1}{2}\times8e$	$4b$; $\frac{p-1}{2}\times8e$	$4c(d^*)$; $\frac{p-1}{2}\times8e$	$4d(c^*)$; $\frac{p-1}{2}\times8e$	$p\times8e$
	p = prime >2; $u=1,\ldots,p-1$						
[3] $Pccn$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a$; $8e$	$4b$; $8e$	$3\times4c$	$3\times4d$	$3\times8e$
[p] $Pccn$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$4a$; $\frac{p-1}{2}\times8e$	$4b$; $\frac{p-1}{2}\times8e$	$p\times4c$	$p\times4d$	$p\times8e$
	p = prime >2; $u=1,\ldots,p-1$						

* $p=4n-1$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pnaa$	$a\to b$; $c\to a$	$\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$	$x\to y\to z\to x$
$Pbnb$	$a\to c$; $c\to b$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

D_{2h}^{11} $P2/b2_1/c2_1/m$ No. 57 $Pbcm$

	Axes	Coordinates	Wyckoff positions 4a	4b	4c	4d	8e
I Maximal *translationengleiche* subgroups							
[2] $Pbc2_1$ (29)			4a	4a	4a	4a	2×4a
$\widehat{=}$ $Pca2_1$	**b**, **a**, −**c**	$y,x,-z$					
[2] $P2cm$ (28)		$x,y+\frac{1}{4},z$	4d	4d	2a; 2b	2×2c	2×4d
$\widehat{=}$ $Pma2$	**c**, **b**, −**a**	$z,y+\frac{1}{4},-x$					
[2] $Pb2_1m$ (26)		$x,y,z+\frac{1}{4}$	4c	4c	4c	2a; 2b	2×4c
$\widehat{=}$ $Pmc2_1$	**c**, **a**, **b**	$z+\frac{1}{4},x,y$					
[2] $P22_12_1$ (18)		$x,y+\frac{1}{4},z$	4c	4c	2a; 2b	4c	2×4c
$\widehat{=}$ $P2_12_12$	**b**, **c**, **a**	$y+\frac{1}{4},z,x$					
[2] $P12_1/c1$ (14)			2a; 2c	2b; 2d	4e	4e	2×4e
[2] $P2/b11$ (13)			2a; 2d	2b; 2c	2e; 2f	4g	2×4g
$\widehat{=}$ $P12/c1$	**c**, **a**, **b**	z,x,y					
[2] $P112_1/m$ (11)			2a; 2b	2c; 2d	4f	2×2e	2×4f
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, non-isomorphic							
[2] $Pbnm$ (62)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z$; $+(\frac{1}{2},0,0)$	4a; 4b	8d	8d	2×4c	2×8d
$\widehat{=}$ $Pnma$	**b**, **c**, 2**a**	$y,z,\frac{1}{2}x$; $+(0,0,\frac{1}{2})$					
[2] $Pbnm$ (62)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z$; $+(\frac{1}{2},0,0)$	8d	4a; 4b	8d	2×4c	2×8d
$\widehat{=}$ $Pnma$	**b**, **c**, 2**a**	$y,z,\frac{1}{2}x+\frac{1}{4}$; $+(0,0,\frac{1}{2})$					
[2] $Pbca$ (61)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z$; $+(\frac{1}{2},0,0)$	4a; 4b	8c	8c	8c	2×8c
[2] $Pbca$ (61)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z$; $+(\frac{1}{2},0,0)$	8c	4a; 4b	8c	8c	2×8c
[2] $Pbna$ (60)	2**a**, **b**, **c**	$\frac{1}{2}x,y,z$; $+(\frac{1}{2},0,0)$	4a; 4b	8d	2×4c	8d	2×8d
$\widehat{=}$ $Pbcn$	**c**, 2**a**, **b**	$z,\frac{1}{2}x,y$; $+(0,\frac{1}{2},0)$					
[2] $Pbna$ (60)	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z$; $+(\frac{1}{2},0,0)$	8d	4a; 4b	2×4c	8d	2×8d
$\widehat{=}$ $Pbcn$	**c**, 2**a**, **b**	$z,\frac{1}{2}x+\frac{1}{4},y$; $+(0,\frac{1}{2},0)$					
Enlarged unit cell, isomorphic							
[2] $Pbcm$	2**a**, **b**, **c**	$\frac{1}{2}x,y,z$; $+(\frac{1}{2},0,0)$	4a; 4b	8e	2×4c	2×4d	2×8e
[2] $Pbcm$	2**a**, **b**, **c**	$\frac{1}{2}x+\frac{1}{4},y,z$; $+(\frac{1}{2},0,0)$	8e	4a; 4b	2×4c	2×4d	2×8e
[3] $Pbcm$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	4a; 8e	4b; 8e	3×4c	3×4d	3×8e
[p] $Pbcm$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$	4a; $\frac{p-1}{2}$×8e	4b; $\frac{p-1}{2}$×8e	p×4c	p×4d	p×8e
	p = prime > 2; $u = 1,\ldots,p-1$						
[3] $Pbcm$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	4a; 8e	4b; 8e	4c; 8e	3×4d	3×8e
[p] $Pbcm$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	4a; $\frac{p-1}{2}$×8e	4b; $\frac{p-1}{2}$×8e	4c; $\frac{p-1}{2}$×8e	p×4d	p×8e
	p = prime > 2; $u = 1,\ldots,p-1$						
[3] $Pbcm$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	4a; 8e	4b; 8e	4c; 8e	4d; 8e	3×8e
[p] $Pbcm$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	4a; $\frac{p-1}{2}$×8e	4b; $\frac{p-1}{2}$×8e	4c; $\frac{p-1}{2}$×8e	4d; $\frac{p-1}{2}$×8e	p×8e
	p = prime > 2; $u = 1,\ldots,p-1$						

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pmca$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Pbma$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
$Pcam$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
$Pmab$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
$Pcmb$	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

Pnnm No. 58 $P\,2_1/n\,2_1/n\,2/m$ D_{2h}^{12}

	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$8h$
I Maximal *translationengleiche* subgroups										
[2] $Pnn2$ (34)			$2a$	$2a$	$2b$	$2b$	$2\times 2a$	$2\times 2b$	$4c$	$2\times 4c$
[2] $P2_1nm$ (31) $\widehat{=}\ Pmn2_1$	 **c**, **b**, −**a**	$x, y+\frac{1}{4}, z$ $z, y+\frac{1}{4}, -x$	$2a$	$2a$	$2a$	$2a$	$4b$	$4b$	$2\times 2a$	$2\times 4b$
[2] $Pn2_1m$ (31) $\widehat{=}\ Pmn2_1$	 **c**, **a**, **b**	$x+\frac{1}{4}, y, z$ $z, x+\frac{1}{4}, y$	$2a$	$2a$	$2a$	$2a$	$4b$	$4b$	$2\times 2a$	$2\times 4b$
[2] $P2_12_12$ (18)		$x, y, z+\frac{1}{4}$	$2a$	$2a$	$2b$	$2b$	$2\times 2a$	$2\times 2b$	$4c$	$2\times 4c$
[2] $P12_1/n1$ (14)			$2a$	$2b$	$2c$	$2d$	$4e$	$4e$	$4e$	$2\times 4e$
[2] $P2_1/n11$ (14) $\widehat{=}\ P12_1/n1$	 **c**, **a**, **b**	 z, x, y	$2a$	$2d$	$2b$	$2c$	$4e$	$4e$	$4e$	$2\times 4e$
[2] $P112/m$ (10)			$1a$; $1h$	$1b$; $1g$	$1d$; $1f$	$1c$; $1e$	$2i$; $2l$	$2j$; $2k$	$2m$; $2n$	$2\times 4o$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, isomorphic										
[3] $Pnnm$	3**a**, **b**, **c**	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$2a$; $4g$	$2b$; $4g$	$2c$; $4g$	$2d$; $4g$	$4e$; $8h$	$4f$; $8h$	$3\times 4g$	$3\times 8h$
[p] $Pnnm$ p = prime > 2; $u = 1, \ldots, p-1$	p**a**, **b**, **c**	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$2a$; $\frac{p-1}{2}\times 4g$	$2b$; $\frac{p-1}{2}\times 4g$	$2c$; $\frac{p-1}{2}\times 4g$	$2d$; $\frac{p-1}{2}\times 4g$	$4e$; $\frac{p-1}{2}\times 8h$	$4f$; $\frac{p-1}{2}\times 8h$	$p\times 4g$	$p\times 8h$
[3] $Pnnm$	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$2a$; $4g$	$2b$; $4g$	$2c$; $4g$	$2d$; $4g$	$4e$; $8h$	$4f$; $8h$	$3\times 4g$	$3\times 8h$
[p] $Pnnm$ p = prime > 2; $u = 1, \ldots, p-1$	**a**, p**b**, **c**	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$2a$; $\frac{p-1}{2}\times 4g$	$2b$; $\frac{p-1}{2}\times 4g$	$2c$; $\frac{p-1}{2}\times 4g$	$2d$; $\frac{p-1}{2}\times 4g$	$4e$; $\frac{p-1}{2}\times 8h$	$4f$; $\frac{p-1}{2}\times 8h$	$p\times 4g$	$p\times 8h$
[3] $Pnnm$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$2a$; $4e$	$2b$; $4e$	$2c$; $4f$	$2d$; $4f$	$3\times 4e$	$3\times 4f$	$4g$; $8h$	$3\times 8h$
[p] $Pnnm$ p = prime > 2; $u = 1, \ldots, p-1$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$2a$; $\frac{p-1}{2}\times 4e$	$2b$; $\frac{p-1}{2}\times 4e$	$2c$; $\frac{p-1}{2}\times 4f$	$2d$; $\frac{p-1}{2}\times 4f$	$p\times 4e$	$p\times 4f$	$4g$; $\frac{p-1}{2}\times 8h$	$p\times 8h$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Pmnn **a** → **b** → **c** → **a** $x \to y \to z \to x$

Pnmn **a** ← **b** ← **c** ← **a** $x \leftarrow y \leftarrow z \leftarrow x$

D_{2h}^{13} $\quad P2_1/m2_1/m2/n$ $\quad$ No. 59 $\quad Pmmn$

I Maximal *translationengleiche* subgroups

Subgroup	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$4c$	$4d$	$4e$	$4f$	$8g$
[2] $Pm2_1n$ (31)			$x+\frac{1}{4},y,z$	$2a$	$2a$	$4b$	$4b$	$2\times2a$	$4b$	$2\times4b$
$\widehat{=}\ Pmn2_1$	$\mathbf{a},\mathbf{c},-\mathbf{b}$	$x,z,-y$	$x+\frac{1}{4},z,-y$							
[2] $P2_1mn$ (31)			$x,y+\frac{1}{4},z$	$2a$	$2a$	$4b$	$4b$	$4b$	$2\times2a$	$2\times4b$
$\widehat{=}\ Pmn2_1$	$\mathbf{b},\mathbf{c},\mathbf{a}$	y,z,x	$y+\frac{1}{4},z,x$							
[2] $Pmm2$ (25)			$x+\frac{1}{4},y+\frac{1}{4},z$	$1a;1d$	$1b;1c$	$4i$	$4i$	$2g;2h$	$2e;2f$	$2\times4i$
[2] $P2_12_12$ (18)			$x+\frac{1}{4},y+\frac{1}{4},z$	$2a$	$2b$	$4c$	$4c$	$4c$	$4c$	$2\times4c$
[2] $P112/n$ (13)		$x+\frac{1}{4},y+\frac{1}{4},z$		$2e$	$2f$	$2a;2d$	$2b;2c$	$4g$	$4g$	$2\times4g$
[2] $P2_1/m11$ (11)		$x+\frac{1}{4},y+\frac{1}{4},z$		$2e$	$2e$	$2a;2c$	$2b;2d$	$2\times2e$	$4f$	$2\times4f$
$\widehat{=}\ P12_1/m1$	$\mathbf{c},\mathbf{a},\mathbf{b}$	$z,x+\frac{1}{4},y+\frac{1}{4}$	z,x,y							
[2] $P12_1/m1$ (11)		$x+\frac{1}{4},y+\frac{1}{4},z$		$2e$	$2e$	$2a;2b$	$2c;2d$	$4f$	$2\times2e$	$2\times4f$

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

Subgroup	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$4c$	$4d$	$4e$	$4f$	$8g$
[2] $Pcmn$ (62)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4c$	$4c$	$4a;4b$	$8d$	$8d$	$2\times4c$	$2\times8d$
$\widehat{=}\ Pnma$	$2\mathbf{c},\mathbf{b},-\mathbf{a}$	$\frac{1}{2}z,y+\frac{1}{4},\frac{3}{4}-x;\ +(\frac{1}{2},0,0)$	$\frac{1}{2}z,y,-x;\ +(\frac{1}{2},0,0)$							
[2] $Pcmn$ (62)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4c$	$4c$	$8d$	$4a;4b$	$8d$	$2\times4c$	$2\times8d$
$\widehat{=}\ Pnma$	$2\mathbf{c},\mathbf{b},-\mathbf{a}$	$\frac{1}{2}z+\frac{1}{4},y+\frac{1}{4},\frac{3}{4}-x;+(\frac{1}{2},0,0)$	$\frac{1}{2}z+\frac{1}{4},y,-x;+(\frac{1}{2},0,0)$							
[2] $Pmcn$ (62)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4c$	$4c$	$4a;4b$	$8d$	$2\times4c$	$8d$	$2\times8d$
$\widehat{=}\ Pnma$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	$\frac{1}{2}z,x+\frac{1}{4},y+\frac{1}{4};\ +(\frac{1}{2},0,0)$	$\frac{1}{2}z,x,y;\ +(\frac{1}{2},0,0)$							
[2] $Pmcn$ (62)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4c$	$4c$	$8d$	$4a;4b$	$2\times4c$	$8d$	$2\times8d$
$\widehat{=}\ Pnma$	$2\mathbf{c},\mathbf{a},\mathbf{b}$	$\frac{1}{2}z+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4};+(\frac{1}{2},0,0)$	$\frac{1}{2}z+\frac{1}{4},x,y;+(\frac{1}{2},0,0)$							
[2] $Pccn$ (56)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4c$	$4d$	$4a;4b$	$8e$	$8e$	$8e$	$2\times8e$
[2] $Pccn$ (56)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4c$	$4d$	$8e$	$4a;4b$	$8e$	$8e$	$2\times8e$

Enlarged unit cell, isomorphic

Subgroup	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$4c$	$4d$	$4e$	$4f$	$8g$
[3] $Pmmn$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$2a(b^*)$; $4f$	$2b(a^*)$; $4f$	$4c;8g$	$4d;8g$	$4e;8g$	$3\times4f$	$3\times8g$
[p] $Pmmn$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$ $p=\text{prime}>2;\quad u=1,\ldots,p-1$	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$	$2a(b^\dagger)$; $\frac{p-1}{2}\times4f$	$2b(a^\dagger)$; $\frac{p-1}{2}\times4f$	$4c$; $\frac{p-1}{2}\times8g$	$4d$; $\frac{p-1}{2}\times8g$	$4e$; $\frac{p-1}{2}\times8g$	$p\times4f$	$p\times8g$
[3] $Pmmn$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$2a(b^*)$; $4e$	$2b(a^*)$; $4e$	$4c;8g$	$4d;8g$	$3\times4e$	$4f;8g$	$3\times8g$
[p] $Pmmn$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$ $p=\text{prime}>2;\quad u=1,\ldots,p-1$	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$	$2a(b^\dagger)$; $\frac{p-1}{2}\times4e$	$2b(a^\dagger)$; $\frac{p-1}{2}\times4e$	$4c$; $\frac{p-1}{2}\times8g$	$4d$; $\frac{p-1}{2}\times8g$	$p\times4e$	$4f$; $\frac{p-1}{2}\times8g$	$p\times8g$
[2] $Pmmn$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2\times2a$	$2\times2b$	$4c;4d$	$8g$	$2\times4e$	$2\times4f$	$2\times8g$
[2] $Pmmn$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$2\times2a$	$2\times2b$	$8g$	$4c;4d$	$2\times4e$	$2\times4f$	$2\times8g$
[3] $Pmmn$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$4c;8g$	$4d;8g$	$3\times4e$	$3\times4f$	$3\times8g$
[p] $Pmmn$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}>2;\quad u=1,\ldots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times2a$	$p\times2b$	$4c$; $\frac{p-1}{2}\times8g$	$4d$; $\frac{p-1}{2}\times8g$	$p\times4e$;	$p\times4f$	$p\times8g$

* origin 2
† origin 2 and $p=4n-1$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pnmm$	$a\to b;\ c\to a$	$\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$	$x\to y\to z\to x$
$Pmnm$	$a\to c;\ c\to b$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

$Pbcn$ No. 60 $P2_1/b2/c2_1/n$ D_{2h}^{14}

	Axes	Coordinates	Wyckoff positions 4a	4b	4c	8d
I Maximal *translationengleiche* subgroups						
[2] $P2_1cn$ (33)		$x,y+\frac{1}{4},z$	4a	4a	4a	2×4a
$\widehat{=} Pna2_1$	**c**, **b**, −**a**	$z,y+\frac{1}{4},-x$				
[2] $Pb2n$ (30)		$x,y,z+\frac{1}{4}$	4c	4c	2a; 2b	2×4c
$\widehat{=} Pnc2$	**c**, **a**, **b**	$z+\frac{1}{4},x,y$				
[2] $Pbc2_1$ (29)		$x+\frac{1}{4},y+\frac{1}{4},z$	4a	4a	4a	2×4a
$\widehat{=} Pca2_1$	**b**, **a**, −**c**	$y+\frac{1}{4},x+\frac{1}{4},-z$				
[2] $P2_122_1$ (18)		$x,y+\frac{1}{4},z+\frac{1}{4}$	4c	4c	2a; 2b	2×4c
$\widehat{=} P2_12_12$	**c**, **a**, **b**	$z+\frac{1}{4},x,y+\frac{1}{4}$				
[2] $P2_1/b11$ (14)			2a; 2b	2c; 2d	4e	2×4e
$\widehat{=} P12_1/c1$	**c**, **a**, **b**	z,x,y				
[2] $P112_1/n$ (14)			2a; 2c	2b; 2d	4e	2×4e
[2] $P12/c1$ (13)			2a; 2b	2c; 2d	2e; 2f	2×4g
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[3] $Pbcn$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	4a; 8d	4b; 8d	4c; 8d	3×8d
[p] $Pbcn$	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	4a; $\frac{p-1}{2}$×8d	4b; $\frac{p-1}{2}$×8d	4c; $\frac{p-1}{2}$×8d	p×8d
	$p =$ prime > 2; $u = 1,\ldots,p-1$					
[3] $Pbcn$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	4a; 8d	4b; 8d	3×4c	3×8d
[p] $Pbcn$	**a**, p**b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	4a; $\frac{p-1}{2}$×8d	4b; $\frac{p-1}{2}$×8d	p×4c	p×8d
	$p =$ prime > 2; $u = 1,\ldots,p-1$					
[3] $Pbcn$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	4a; 8d	4b; 8d	4c; 8d	3×8d
[p] $Pbcn$	**a**, **b**, p**c**	$x,y,\frac{1}{p}x;\ +(0,0,\frac{u}{p})$	4a; $\frac{p-1}{2}$×8d	4b; $\frac{p-1}{2}$×8d	4c; $\frac{p-1}{2}$×8d	p×8d
	$p =$ prime > 2; $u = 1,\ldots,p-1$					

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pnca$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Pbna$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
$Pcan$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
$Pnab$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
$Pcnb$	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

D_{2h}^{15} $P2_1/b2_1/c2_1/a$ No. 61 $Pbca$

	Axes	Coordinates	Wyckoff positions		
			$4a$	$4b$	$8c$
I Maximal *translationengleiche* subgroups					
[2] $P2_1ca$ (29)		$x, y+\frac{1}{4}, z$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $Pca2_1$	$\mathbf{c}, \mathbf{b}, -\mathbf{a}$	$z, y+\frac{1}{4}, -x$			
[2] $Pb2_1a$ (29)		$x, y, z+\frac{1}{4}$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $Pca2_1$	$\mathbf{a}, \mathbf{c}, -\mathbf{b}$	$x, z+\frac{1}{4}, -y$			
[2] $Pbc2_1$ (29)		$x+\frac{1}{4}, y, z$	$4a$	$4a$	$2\times4a$
$\widehat{=}$ $Pca2_1$	$\mathbf{b}, \mathbf{a}, -\mathbf{c}$	$y, x+\frac{1}{4}, -z$			
[2] $P2_12_12_1$ (19)			$4a$	$4a$	$2\times4a$
[2] $P2_1/b11$ (14)			$2a; 2d$	$2b; 2c$	$2\times4e$
$\widehat{=}$ $P12_1/c1$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y			
[2] $P12_1/c1$ (14)			$2a; 2d$	$2b; 2c$	$2\times4e$
[2] $P112_1/a$ (14)			$2a; 2d$	$2b; 2c$	$2\times4e$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, isomorphic					
[3] $Pbca$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	$4a; 8c$	$4b; 8c$	$3\times8c$
[p] $Pbca$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$4a; \frac{p-1}{2}\times8c$	$4b; \frac{p-1}{2}\times8c$	$p\times8c$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$				
[3] $Pbca$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	$4a; 8c$	$4b; 8c$	$3\times8c$
[p] $Pbca$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$4a; \frac{p-1}{2}\times8c$	$4b; \frac{p-1}{2}\times8c$	$p\times8c$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$				
[3] $Pbca$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$4a; 8c$	$4b; 8c$	$3\times8c$
[p] $Pbca$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$4a; \frac{p-1}{2}\times8c$	$4b; \frac{p-1}{2}\times8c$	$p\times8c$
	$p = \text{prime} > 2;\ u = 1, \ldots, p-1$				

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Pcab$ $a \rightleftarrows b$ $\mathbf{a} \rightleftarrows -\mathbf{b}$ $x \rightleftarrows -y$

Pnma No. 62 $P2_1/n2_1/m2_1/a$ D_{2h}^{16}

	Axes	Coordinates	Wyckoff positions 4*a*	4*b*	4*c*	8*d*
I Maximal *translationengleiche* subgroups						
[2] $Pn2_1a$ (33)			4*a*	4*a*	4*a*	2×4*a*
$\widehat{=}$ $Pna2_1$	**a**, **c**, −**b**	$x, z, -y$				
[2] $Pnm2_1$ (31)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	4*b*	4*b*	2×2*a*	2×4*b*
$\widehat{=}$ $Pmn2_1$	**b**, **a**, −**c**	$y+\frac{1}{4}, x+\frac{1}{4}, -z$				
[2] $P2_1ma$ (26)		$x, y+\frac{1}{4}, z+\frac{1}{4}$	4*c*	4*c*	2*a*; 2*b*	2×4*c*
$\widehat{=}$ $Pmc2_1$	**b**, **c**, **a**	$y+\frac{1}{4}, z+\frac{1}{4}, x$				
[2] $P2_12_12_1$ (19)		$x, y, z+\frac{1}{4}$	4*a*	4*a*	4*a*	2×4*a*
[2] $P2_1/n11$ (14)			2*a*; 2*b*	2*c*; 2*d*	4*e*	2×4*e*
$\widehat{=}$ $P12_1/n1$	**c**, **a**, **b**	z, x, y				
[2] $P112_1/a$ (14)			2*a*; 2*b*	2*c*; 2*d*	4*e*	2×4*e*
[2] $P12_1/m1$ (11)			2*a*; 2*d*	2*b*; 2*c*	2×2*e*	2×4*f*
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[3] *Pnma*	3**a**, **b**, **c**	$\frac{1}{3}x, y, z; \pm(\frac{1}{3}, 0, 0)$	4*a*; 8*d*	4*b*; 8*d*	3×4*c*	3×8*d*
[*p*] *Pnma*	*p***a**, **b**, **c**	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	4*a*; $\frac{p-1}{2}$×8*d*	4*b*; $\frac{p-1}{2}$×8*d*	*p*×4*c*	*p*×8*d*
	p = prime > 2; $u = 1, \ldots, p-1$					
[3] *Pnma*	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z; \pm(0, \frac{1}{3}, 0)$	4*a*; 8*d*	4*b*; 8*d*	4*c*; 8*d*	3×8*d*
[*p*] *Pnma*	**a**, *p***b**, **c**	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	4*a*; $\frac{p-1}{2}$×8*d*	4*b*; $\frac{p-1}{2}$×8*d*	4*c*; $\frac{p-1}{2}$×8*d*	*p*×8*d*
	p = prime > 2; $u = 1, \ldots, p-1$					
[3] *Pnma*	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	4*a*; 8*d*	4*b*; 8*d*	3×4*c*	3×8*d*
[*p*] *Pnma*	**a**, **b**, *p***c**	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	4*a*; $\frac{p-1}{2}$×8*d*	4*b*; $\frac{p-1}{2}$×8*d*	*p*×4*c*	*p*×8*d*
	p = prime > 2; $u = 1, \ldots, p-1$					

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Pbnm	$a \to b$; $c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
Pmcn	$a \to c$; $c \to b$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
Pmnb	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
Pcmn	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
Pnam	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

Cmcm No. 63 $C2/m2/c2_1/m$ CONTINUED (*from next page*)

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Amma	$C \to A$; $A \to B$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
Bbmm	$C \to B$; $A \to C$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$
Ccmm	$A \to B$	$a \rightleftarrows b$	$\mathbf{a} \rightleftarrows -\mathbf{b}$	$x \rightleftarrows -y$
Amam	$C \rightleftarrows A$	$a \rightleftarrows c$	$\mathbf{a} \rightleftarrows -\mathbf{c}$	$x \rightleftarrows -z$
Bmmb	$C \to B$	$b \rightleftarrows c$	$\mathbf{b} \rightleftarrows -\mathbf{c}$	$y \rightleftarrows -z$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 63, pp. 530–531.

D_{2h}^{17} $C\,2/m\,2/c\,2_1/m$ No. 63 $C\,m\,c\,m$

	Axes	Coordinates	Wyckoff positions 4a	4b	4c	8d	8e	8f	8g	16h
I Maximal *translationengleiche* subgroups										
[2] *C*2*cm* (40)			4*a*	4*a*	4*b*	8*c*	2×4*a*	8*c*	2×4*b*	2×8*c*
≙ *Ama*2	**c**, **b**, −**a**	*z*, *y*, −*x*								
[2] *Cm*2*m* (38)		$x, y, z+\frac{1}{4}$	4*c*	4*c*	2*a*; 2*b*	8*f*	8*f*	2×4*c*	4*d*; 4*e*	2×8*f*
≙ *Amm*2	**c**, **a**, **b**	$z+\frac{1}{4}, x, y$								
[2] $Cmc2_1$ (36)			4*a*	4*a*	4*a*	8*b*	8*b*	2×4*a*	8*b*	2×8*b*
[2] $C222_1$ (20)			4*a*	4*a*	4*b*	8*c*	2×4*a*	8*c*	8*c*	2×8*c*
[2] *C*12/*c*1 (15)			4*a*	4*b*	4*e*	4*c*; 4*d*	8*f*	8*f*	8*f*	2×8*f*
[2] *C*2/*m*11 (12)			2*a*; 2*c*	2*b*; 2*d*	4*i*	4*e*; 4*f*	4*g*; 4*h*	2×4*i*	8*j*	2×8*j*
≙ *C*12/*m*1	**b**, −**a**, **c**	*y*, −*x*, *z*								
[2] $P112_1/m$	**a**, $\frac{1}{2}$(−**a**+**b**), **c**	*x*+*y*, 2*y*, *z*	2*a*	2*c*	2*e*	2*b*; 2*d*	4*f*	4*f*	2×2*e*	2×4*f*
(11)	or: $\frac{1}{2}$(**a**−**b**), **b**, **c**	2*x*, *x*+*y*, *z*	2*a*	2*b*	2*e*	2*c*; 2*d*	4*f*	4*f*	2×2*e*	2×4*f*
	or: $\frac{1}{2}$(**a**−**b**), $\frac{1}{2}$(**a**+**b**), **c**	*x*−*y*, *x*+*y*, *z*	2*a*	2*d*	2*e*	2*b*; 2*c*	4*f*	4*f*	2×2*e*	2×4*f*
II Maximal *klassengleiche* subgroups										
Loss of centring translations										
[2] *Pbnm* (62)			4*a*	4*b*	4*c*	8*d*	8*d*	8*d*	2×4*c*	2×8*d*
≙ *Pnma*	**b**, **c**, **a**	*y*, *z*, *x*								
[2] *Pmcn* (62)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	4*c*	4*c*	4*c*	4*a*; 4*b*	8*d*	2×4*c*	8*d*	2×8*d*
≙ *Pnma*	**c**, **a**, **b**	$z, x+\frac{1}{4}, y+\frac{1}{4}$								
[2] *Pbcn* (60)			4*a*	4*b*	4*c*	8*d*	8*d*	8*d*	8*d*	2×8*d*
[2] *Pmnm* (59)		origin 1: $x, y+\frac{1}{4}, z+\frac{1}{4}$ origin 2: $x-\frac{1}{4}, y+\frac{1}{4}, z$	4*f*	4*f*	2*a*; 2*b*	4*c*; 4*d*	8*g*	2×4*f*	2×4*e*	2×8*g*
≙ *Pmmn*	**c**, **a**, **b**	$z+\frac{1}{4}, x, y+\frac{1}{4}$ (origin 1) $z, x-\frac{1}{4}, y+\frac{1}{4}$ (origin 2)								
[2] *Pmnn* (58)			2*a*; 2*c*	2*b*; 2*d*	4*g*	8*h*	4*e*; 4*f*	2×4*g*	8*h*	2×8*h*
≙ *Pnnm*	**b**, **c**, **a**	*y*, *z*, *x*								
[2] *Pbcm* (57)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	4*c*	4*c*	4*d*	4*a*; 4*b*	2×4*c*	8*e*	2×4*d*	2×8*e*
[2] *Pbnn* (52)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	4*c*	4*c*	4*d*	4*a*; 4*b*	2×4*c*	8*e*	8*e*	2×8*e*
≙ *Pnna*	**b**, **c**, **a**	$y+\frac{1}{4}, z, x+\frac{1}{4}$								
[2] *Pmcm* (51)			2*a*; 2*d*	2*b*; 2*c*	2*e*; 2*f*	8*l*	4*g*; 4*h*	4*i*; 4*j*	2×4*k*	2×8*l*
≙ *Pmma*	**c**, **a**, **b**	*z*, *x*, *y*								
Enlarged unit cell, isomorphic										
[3] *Cmcm*	3**a**, **b**, **c**	$\frac{1}{3}x, y, z$; $\pm(\frac{1}{3}, 0, 0)$	4*a*; 8*e*	4*b*; 8*e*	4*c*; 8*g*	8*d*; 16*h*	3×8*e*	8*f*; 16*h*	3×8*g*	3×16*h*
[*p*] *Cmcm*	*p***a**, **b**, **c**	$\frac{1}{3}x, y, z$; $+(\frac{u}{p}, 0, 0)$ *p* = prime > 2; *u* = 1, …, *p*−1	4*a*; $\frac{p-1}{2}$×8*e*	4*b*; $\frac{p-1}{2}$×8*e*	4*c*; $\frac{p-1}{2}$×8*g*	8*d*; $\frac{p-1}{2}$×16*h*	*p*×8*e*	8*f*; $\frac{p-1}{2}$×16*h*	*p*×8*g*	*p*×16*h*
[3] *Cmcm*	**a**, 3**b**, **c**	$x, \frac{1}{3}y, z$; $\pm(0, \frac{1}{3}, 0)$	4*a*; 8*f*	4*b*; 8*f*	3×4*c*	8*d*; 16*h*	8*e*; 16*h*	3×8*f*	3×8*g*	3×16*h*
[*p*] *Cmcm*	**a**, *p***b**, **c**	$x, \frac{1}{p}y, z$; $+(0, \frac{u}{p}, 0)$ *p* = prime > 2; *u* = 1, …, *p*−1	4*a*; $\frac{p-1}{2}$×8*f*	4*b*; $\frac{p-1}{2}$×8*f*	*p*×4*c*	8*d*; $\frac{p-1}{2}$×16*h*	8*e*; $\frac{p-1}{2}$×16*h*	*p*×8*f*	*p*×8*g*	*p*×16*h*
[3] *Cmcm*	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	4*a*; 8*f*	4*b*; 8*f*	4*c*; 8*f*	8*d*; 16*h*	8*e*; 16*h*	3×8*f*	8*g*; 16*h*	3×16*h*
[*p*] *Cmcm*	**a**, **b**, *p***c**	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$ *p* = prime > 2; *u* = 1, …, *p*−1	4*a*; $\frac{p-1}{2}$×8*f*	4*b*; $\frac{p-1}{2}$×8*f*	4*c*; $\frac{p-1}{2}$×8*f*	8*d*; $\frac{p-1}{2}$×16*h*	8*e*; $\frac{p-1}{2}$×16*h*	*p*×8*f*	8*g*; $\frac{p-1}{2}$×16*h*	*p*×16*h*

Continued on preceding page

Cmce No. 64 $C2/m2/c2_1/e$ D_{2h}^{18}

	Axes	Coordinates	4*a*	4*b*	8*c*	8*d*	8*e*	8*f*	16*g*
I Maximal *translationengleiche* subgroups									
[2] *C*2*ce* (41)			4*a*	4*a*	8*b*	2×4*a*	8*b*	8*b*	2×8*b*
≘ *Aea*2	**c**, −**b**, **a**	$z,-y,x$							
[2] *Cm*2*e* (39)		$x+\frac{1}{4},y,z+\frac{1}{4}$	4*c*	4*c*	8*d*	8*d*	4*a*; 4*b*	2×4*c*	2×8*d*
≘ *Aem*2	**c**, **a**, **b**	$z+\frac{1}{4},x+\frac{1}{4},y$							
[2] $Cmc2_1$ (36)		$x,y+\frac{1}{4},z$	4*a*	4*a*	8*b*	8*b*	8*b*	2×4*a*	2×8*b*
[2] $C222_1$ (20)		$x+\frac{1}{4},y,z$	4*a*	4*a*	8*c*	2×4*a*	2×4*b*	8*c*	2×8*c*
[2] $C2/m11$ (12)			2*a*; 2*d*	2*b*; 2*c*	4*e*; 4*f*	4*g*; 4*h*	8*j*	2×4*i*	2×8*j*
≘ $C12/m1$	**b**, −**a**, **c**	$y,-x,z$							
[2] $C12/c1$ (15)		$x+\frac{1}{4},y+\frac{1}{4},z$	4*c*	4*d*	4*a*; 4*b*	8*f*	2×4*e*	8*f*	2×8*f*
[2] $P112_1/a$ (14)	**a**, $\frac{1}{2}$(−**a**+**b**), **c**	$x+y,2y,z$	2*a*	2*c*	2*b*; 2*d*	4*e*	4*e*	4*e*	2×4*e*
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] *Pmnb* (62)		$x+\frac{1}{4},y+\frac{1}{4},z$	4*c*	4*c*	4*a*; 4*b*	8*d*	8*d*	2×4*c*	2×8*d*
≘ *Pnma*	**b**, −**a**, **c**	$y+\frac{1}{4},-x-\frac{1}{4},z$							
[2] *Pbca* (61)			4*a*	4*b*	8*c*	8*c*	8*c*	8*c*	2×8*c*
[2] *Pbna* (60)		$x+\frac{1}{4},y+\frac{1}{4},z$	4*c*	4*c*	4*a*; 4*b*	2×4*c*	8*d*	8*d*	2×8*d*
≘ *Pbcn*	**c**, **a**, **b**	$z,x+\frac{1}{4},y+\frac{1}{4}$							
[2] *Pmca* (57)		$x+\frac{1}{4},y+\frac{1}{4},z$	4*d*	4*d*	4*a*; 4*b*	8*e*	2×4*c*	2×4*d*	2×8*e*
≘ *Pbcm*	**b**, **c**, **a**	$y+\frac{1}{4},z,x+\frac{1}{4}$							
[2] *Pbnb* (56)			4*a*	4*b*	8*e*	8*e*	4*c*; 4*d*	8*e*	2×8*e*
≘ *Pccn*	**c**, **a**, **b**	z,x,y							
[2] *Pmcb* (55)			2*a*; 2*d*	2*b*; 2*c*	8*i*	4*e*; 4*f*	8*i*	4*g*; 4*h*	2×8*i*
≘ *Pbam*	**b**, **c**, **a**	y,z,x							
[2] *Pbcb* (54)		$x+\frac{1}{4},y+\frac{1}{4},z$	4*c*	4*c*	4*a*; 4*b*	2×4*c*	4*d*; 4*e*	8*f*	2×8*f*
≘ *Pcca*	**c**, **a**, **b**	$z,x+\frac{1}{4},y+\frac{1}{4}$							
[2] *Pmna* (53)			2*a*; 2*c*	2*b*; 2*d*	8*i*	4*e*; 4*f*	2×4*g*	2×4*h*	2×8*i*
Enlarged unit cell, isomorphic									
[3] *Cmce*	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	4*a*; 8*d*	4*b*; 8*d*	8*c*; 16*g*	3×8*d*	8*e*; 16*g*	8*f*; 16*g*	3×16*g*
[*p*] *Cmce*	*p***a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	4*a*; $\frac{p-1}{2}\times 8d$	4*b*; $\frac{p-1}{2}\times 8d$	8*c*; $\frac{p-1}{2}\times 16g$	*p*×8*d*	8*e*; $\frac{p-1}{2}\times 16g$	8*f*; $\frac{p-1}{2}\times 16g$	*p*×16*g*
	p = prime > 2; $u=1,\ldots,p-1$								
[3] *Cmce*	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	4*a*; 8*f*	4*b*; 8*f*	8*c*; 16*g*	8*d*; 16*g*	3×8*e*	3×8*f*	3×16*g*
[*p*] *Cmce*	**a**, *p***b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	4*a*; $\frac{p-1}{2}\times 8f$	4*b*; $\frac{p-1}{2}\times 8f$	8*c*; $\frac{p-1}{2}\times 16g$	8*d*; $\frac{p-1}{2}\times 16g$	*p*×8*e*	*p*×8*f*	*p*×16*g*
	p = prime > 2; $u=1,\ldots,p-1$								
[3] *Cmce*	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	4*a*; 8*f*	4*b*; 8*f*	8*c*; 16*g*	8*d*; 16*g*	8*e*; 16*g*	3×8*f*	3×16*g*
[*p*] *Cmce*	**a**, **b**, *p***c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	4*a*; $\frac{p-1}{2}\times 8f$	4*b*; $\frac{p-1}{2}\times 8f$	8*c*; $\frac{p-1}{2}\times 16g$	8*d*; $\frac{p-1}{2}\times 16g$	8*e*; $\frac{p-1}{2}\times 16g$	*p*×8*f*	*p*×16*g*
	p = prime > 2; $u=1,\ldots,p-1$								

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Aema	$C\to A$; $A\to B$	$a\to b\to c\to a$	$\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$	$x\to y\to z\to x$
Bbem	$C\to B$; $A\to C$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$
Ccme	$A\to B$	$a\rightleftarrows b$	$\mathbf{a}\rightleftarrows -\mathbf{b}$	$x\rightleftarrows -y$
Aeam	$A\rightleftarrows C$	$a\rightleftarrows c$	$\mathbf{a}\rightleftarrows -\mathbf{c}$	$x\rightleftarrows -z$
Bmeb	$C\to B$	$b\rightleftarrows c$	$\mathbf{b}\rightleftarrows -\mathbf{c}$	$y\rightleftarrows -z$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 65, pp. 533–535.

D_{2h}^{19} $C2/m2/m2/m$ No. 65 $Cmmm$

	Axes	Coordinates	2*a*	2*b*	2*c*	2*d*	4*e*	4*f*	4*g* 8*m*	4*h* 8*n*	4*i* 8*o*	4*j* 8*p*	4*k* 8*q*	4*l* 16*r*
I Maximal *translationengleiche* subgroups														
[2] *C2mm* (38) ≙ *Amm*2	**c**, −**b**, **a**	*z*, −*y*, *x*	2*a*	2*a*	2*b*	2*b*	4*d*	4*e*	2×2*a* 8*f*	2×2*b* 8*f*	4*d* 2×4*c*	4*e* 2×4*d*	4*c* 2×4*e*	4*c* 2×8*f*
[2] *Cm2m* (38) ≙ *Amm*2	**c**, **a**, **b**	*z*, *x*, *y*	2*a*	2*a*	2*b*	2*b*	4*d*	4*e*	4*d* 8*f*	4*e* 2×4*c*	2×2*a* 8*f*	2×2*b* 2×4*d*	4*c* 2×4*e*	4*c* 2×8*f*
[2] *Cmm*2 (35)			2*a*	2*b*	2*b*	2*a*	4*c*	4*c*	4*d* 2×4*c*	4*d* 2×4*e*	4*e* 2×4*d*	4*e* 8*f*	2×2*a* 8*f*	2×2*b* 2×8*f*
[2] *C*222 (21)			2*a*	2*b*	2*c*	2*d*	4*k*	4*k*	4*e* 2×4*k*	4*f* 8*l*	4*g* 8*l*	4*h* 8*l*	4*i* 8*l*	4*j* 2×8*l*
[2] *C*2/*m*11 (12) ≙ *C*12/*m*1	**b**, −**a**, **c**	*y*, −*x*, *z*	2*a*	2*b*	2*d*	2*c*	4*e*	4*f*	4*g* 8*j*	4*h* 2×4*i*	4*i* 8*j*	4*i* 8*j*	4*i* 8*j*	4*i* 2×8*j*
[2] *C*12/*m*1 (12)			2*a*	2*b*	2*d*	2*c*	4*e*	4*f*	4*i* 8*j*	4*i* 8*j*	4*g* 2×4*i*	4*h* 8*j*	4*i* 8*j*	4*i* 2×8*j*
[2] *P*112/*m* (10)	**a**, $\frac{1}{2}$(−**a**+**b**), **c**	*x*+*y*, 2*y*, *z*	1*a*	1*c*	1*f*	1*b*	1*d*; 1*g*	1*e*; 1*h*	2*m* 2*j*; 2*l*	2*n* 4*o*	2*m* 4*o*	2*n* 2×2*m*	2*i* 2×2*n*	2*k* 2×4*o*
	or: $\frac{1}{2}$(**a**−**b**), $\frac{1}{2}$(**a**+**b**), **c**	*x*−*y*, *x*+*y*, *z*	1*a*	1*g*	1*h*	1*b*	1*c*; 1*d*	1*e*; 1*f*	2*m* 2*j*; 2*k*	2*n* 4*o*	2*m* 4*o*	2*n* 2×2*m*	2*i* 2×2*n*	2*l* 2×4*o*
II Maximal *klassengleiche* subgroups **Loss of centring translations**														
[2] *Pmmn* (59)		origin 1: *x*, *y*, *z* origin 2: $x+\frac{1}{4}, y+\frac{1}{4}, z$	2*a*	2*b*	2*b*	2*a*	4*c*	4*d*	4*f* 8*g*	4*f* 2×4*e*	4*e* 2×4*f*	4*e* 8*g*	2×2*a* 8*g*	2×2*b* 2×8*g*
[2] *Pbam* (55)			2*a*	2*c*	2*d*	2*b*	4*g*	4*h*	4*g* 8*i*	4*h* 8*i*	4*g* 8*i*	4*h* 2×4*g*	4*e* 2×4*h*	4*f* 2×8*i*
[2] *Pbmn* (53) ≙ *Pmna*	**b**, **c**, **a**	*y*, *z*, *x*	2*a*	2*b*	2*c*	2*d*	4*g*	4*g*	4*h* 2×4*g*	4*h* 8*i*	4*e* 2×4*h*	4*f* 8*i*	4*h* 8*i*	4*h* 2×8*i*
[2] *Pman* (53) ≙ *Pmna*	**a**, −**c**, **b**	*x*, −*z*, *y*	2*a*	2*b*	2*c*	2*d*	4*g*	4*g*	4*e* 2×4*g*	4*f* 2×4*h*	4*h* 8*i*	4*h* 8*i*	4*h* 8*i*	4*h* 2×8*i*
[2] *Pbmm* (51) ≙ *Pmma*	**b**, **c**, **a**	$x+\frac{1}{4}, y+\frac{1}{4}, z$ $y+\frac{1}{4}, z, x+\frac{1}{4}$	2*e*	2*e*	2*f*	2*f*	2*a*; 2*c*	2*b*; 2*d*	2×2*e* 4*g*; 4*h*	2×2*f* 8*l*	4*i* 2×4*k*	4*j* 2×4*i*	4*k* 2×4*j*	4*k* 2×8*l*
[2] *Pmam* (51) ≙ *Pmma*	**a**, −**c**, **b**	$x+\frac{1}{4}, y+\frac{1}{4}, z$ $x+\frac{1}{4}, -z, y+\frac{1}{4}$	2*e*	2*e*	2*f*	2*f*	2*a*; 2*c*	2*b*; 2*d*	4*i* 4*g*; 4*h*	4*j* 2×4*k*	2×2*e* 8*l*	2×2*f* 2×4*i*	4*k* 2×4*j*	4*k* 2×8*l*
[2] *Pban* (50)		origin 1: *x*, *y*, *z* origin 2: $x+\frac{1}{4}, y+\frac{1}{4}, z$	2*a*	2*b*	2*c*	2*d*	4*e*	4*f*	4*g* 8*m*	4*h* 8*m*	4*i* 8*m*	4*j* 8*m*	4*k* 8*m*	4*l* 2×8*m*
[2] *Pmmm* (47)			1*a*; 1*f*	1*b*; 1*e*	1*d*; 1*g*	1*c*; 1*h*	4*y*	4*z*	2*i*; 2*k* 8α	2*j*; 2*l* 4*u*; 4*v*	2*m*; 2*o* 4*w*; 4*x*	2*n*; 2*p* 2×4*y*	2*q*; 2*t* 2×4*z*	2*r*; 2*s* 2×8α

	Axes	Coordinates	2*a*	2*b*	2*c*	2*d*	4*e*	4*f*	4*g* 8*m*	4*h* 8*n*	4*i* 8*o*	4*j* 8*p*	4*k* 8*q*	4*l* 16*r*
Enlarged unit cell, non-isomorphic														
[2] *Ibmm* (74)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*a*	4*b*	4*e*	4*e*	8*g*	4*c*; 4*d*	8*h* 2×8*g*	2×4*e* 16*j*	8*f* 2×8*h*	8*i* 16*j*	8*h* 2×8*i*	8*h* 2×16*j*
≙ *Imma*	**b**, 2**c**, **a**	$y,\frac{1}{2}z,x$; $+(0,\frac{1}{2},0)$												
[2] *Ibmm* (74)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*e*	4*e*	4*b*	4*a*	4*c*; 4*d*	8*g*	2×4*e* 2×8*g*	8*h* 16*j*	8*i* 2×8*h*	8*f* 2×8*i*	8*h* 16*j*	8*h* 2×16*j*
≙ *Imma*	**b**, 2**c**, **a**	$y,\frac{1}{2}z+\frac{1}{4},x$; $+(0,\frac{1}{2},0)$												
[2] *Imam* (74)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*a*	4*b*	4*e*	4*e*	8*g*	4*c*; 4*d*	8*f* 2×8*g*	8*i* 2×8*h*	8*h* 16*j*	2×4*e* 16*j*	8*h* 2×8*i*	8*h* 2×16*j*
≙ *Imma*	**a**,−2**c**,**b**	$x,-\frac{1}{2}z,y$; $+(0,\frac{1}{2},0)$												
[2] *Imam* (74)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*e*	4*e*	4*b*	4*a*	4*c*; 4*d*	8*g*	8*i* 2×8*g*	8*f* 2×8*h*	2×4*e* 16*j*	8*h* 2×8*i*	8*h* 16*j*	8*h* 2×16*j*
≙ *Imma*	**a**,−2**c**,**b**	$x,-\frac{1}{2}z-\frac{1}{4},y$; $+(0,0,\frac{1}{2})$												
[2] *Ibam* (72)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*c*	4*d*	4*b*	4*a*	8*j*	8*e*	8*j* 16*k*	8*f* 16*k*	8*j* 16*k*	8*g* 2×8*j*	8*h* 16*k*	8*i* 2×16*k*
[2] *Ibam* (72)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*a*	4*b*	4*d*	4*c*	8*e*	8*j*	8*f* 16*k*	8*j* 16*k*	8*g* 16*k*	8*j* 16*k*	8*h* 2×8*j*	8*i* 2×16*k*
[2] *Immm* (71)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*a*; 2*c*	2*b*; 2*d*	4*j*	4*i*	8*n*	8*k*	4*e*; 4*f* 16*o*	8*m* 2×8*l*	4*g*; 4*h* 2×8*m*	8*l* 2×8*n*	2×4*i* 16*o*	2×4*j* 2×16*o*
[2] *Immm* (71)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*i*	4*j*	2*b*; 2*d*	2*a*; 2*c*	8*k*	8*n*	8*m* 16*o*	4*e*; 4*f* 2×8*l*	8*l* 2×8*m*	4*g*; 4*h* 16*o*	2×4*i* 2×8*n*	2×4*j* 2×16*o*
[2] *Cccm* (66)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*c*	4*d*	4*b*	4*a*	4*e*; 4*f*	8*k*	8*l* 2×8*k*	8*g* 16*m*	8*l* 16*m*	8*h* 2×8*l*	8*i* 16*m*	8*j* 2×16*m*
[2] *Cccm* (66)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*a*	4*b*	4*d*	4*c*	8*k*	4*e*; 4*f*	8*g* 2×8*k*	8*l* 16*m*	8*h* 16*m*	8*l* 16*m*	8*i* 2×8*l*	8*j* 2×16*m*
[2] *Ccmm* (63)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*a*	4*b*	4*c*	4*c*	8*d*	8*g*	8*f* 16*h*	2×4*c* 16*h*	8*e* 2×8*f*	8*g* 16*h*	8*f* 2×8*g*	8*f* 2×16*h*
≙ *Cmcm*	**b**, −**a**, 2**c**	$y,-x,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$												
[2] *Ccmm* (63)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*c*	4*c*	4*b*	4*a*	8*g*	8*d*	2×4*c* 16*h*	8*f* 16*h*	8*g* 2×8*f*	8*e* 2×8*g*	8*f* 16*h*	8*f* 2×16*h*
≙ *Cmcm*	**b**, −**a**, 2**c**	$y,-x,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$												
[2] *Cmcm* (63)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*a*	4*b*	4*c*	4*c*	8*d*	8*g*	8*e* 16*h*	8*g* 2×8*f*	8*f* 16*h*	2×4*c* 16*h*	8*f* 2×8*g*	8*f* 2×16*h*
[2] *Cmcm* (63)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*c*	4*c*	4*b*	4*a*	8*g*	8*d*	8*g* 16*h*	8*e* 2×8*f*	2×4*c* 16*h*	8*f* 2×8*g*	8*f* 16*h*	8*f* 2×16*h*

	Axes	Coordinates	Wyckoff positions									
			$2a$	$2b$	$2c$ $4k$	$2d$ $4l$	$4e$ $8m$	$4f$ $8n$	$4g$ $8o$	$4h$ $8p$	$4i$ $8q$	$4j$ $16r$
Enlarged unit cell, isomorphic												
[3] *Cmmm*	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$2a;4g$	$2b;4g$	$2c;4h$ $4k;8o$	$2d;4h$ $4l;8o$	$4e;8p$ $8m;16r$	$4f;8q$ $8n;16r$	$3\times4g$ $3\times8o$	$3\times4h$ $3\times8p$	$4i;8p$ $3\times8q$	$4j;8q$ $3\times16r$
[p] *Cmmm*	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$ $p=$prime >2; $u=1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times4g$	$2b$; $\frac{p-1}{2}\times4g$	$2c$; $\frac{p-1}{2}\times4h$ $4k$; $\frac{p-1}{2}\times8o$	$2d$; $\frac{p-1}{2}\times4h$ $4l$; $\frac{p-1}{2}\times8o$	$4e$; $\frac{p-1}{2}\times8p$ $8m$; $\frac{p-1}{2}\times16r$	$4f$; $\frac{p-1}{2}\times8q$ $8n$; $\frac{p-1}{2}\times16r$	$p\times4g$ $p\times8o$	$p\times4h$ $p\times8p$	$4i$; $\frac{p-1}{2}\times8p$ $p\times8q$	$4j$; $\frac{p-1}{2}\times8q$ $p\times16r$
[3] *Cmmm*	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$2a;4i$	$2b;4i$	$2c;4j$ $4k;8n$	$2d;4j$ $4l;8n$	$4e;8p$ $8m;16r$	$4f;8q$ $3\times8n$	$4g;8p$ $8o;16r$	$4h;8q$ $3\times8p$	$3\times4i$ $3\times8q$	$3\times4j$ $3\times16r$
[p] *Cmmm*	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$ $p=$prime >2; $u=1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times4i$	$2b$; $\frac{p-1}{2}\times4i$	$2c$; $\frac{p-1}{2}\times4j$ $4k$; $\frac{p-1}{2}\times8n$	$2d$; $\frac{p-1}{2}\times4j$ $4l$; $\frac{p-1}{2}\times8n$	$4e$; $\frac{p-1}{2}\times8p$ $8m$; $\frac{p-1}{2}\times16r$	$4f$; $\frac{p-1}{2}\times8q$ $p\times8n$	$4g$; $\frac{p-1}{2}\times8p$ $8o$; $\frac{p-1}{2}\times16r$	$4h$; $\frac{p-1}{2}\times8q$ $p\times8p$	$p\times4i$ $p\times8q$	$p\times4j$ $p\times16r$
[2] *Cmmm*	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a;2d$	$2b;2c$	$4l$ $2\times4k$	$4k$ $2\times4l$	$4e;4f$ $2\times8m$	$8m$ $2\times8n$	$4g;4h$ $2\times8o$	$8o$ $8p;8q$	$4i;4j$ $16r$	$8n$ $2\times16r$
[2] *Cmmm*	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4k$	$4l$	$2b;2c$ $2\times4k$	$2a;2d$ $2\times4l$	$8m$ $2\times8m$	$4e;4f$ $2\times8n$	$8o$ $2\times8o$	$4g;4h$ $16r$	$8n$ $8p;8q$	$4i;4j$ $2\times16r$
[3] *Cmmm*	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a;4k$	$2b;4l$	$2c;4l$ $3\times4k$	$2d;4k$ $3\times4l$	$4e;8m$ $3\times8m$	$4f;8m$ $3\times8n$	$4g;8o$ $3\times8o$	$4h;8o$ $8p;16r$	$4i;8n$ $8q;16r$	$4j;8n$ $3\times16r$
[p] *Cmmm*	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p=$prime >2; $u=1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times4k$	$2b$; $\frac{p-1}{2}\times4l$	$2c$; $\frac{p-1}{2}\times4l$ $p\times4k$	$2d$; $\frac{p-1}{2}\times4k$ $p\times4l$	$4e$; $\frac{p-1}{2}\times8m$ $p\times8m$	$4f$; $\frac{p-1}{2}\times8m$ $p\times8n$	$4g$; $\frac{p-1}{2}\times8o$ $p\times8o$	$4h$; $\frac{p-1}{2}\times8o$ $8p$; $\frac{p-1}{2}\times16r$	$4i$; $\frac{p-1}{2}\times8n$ $8q$; $\frac{p-1}{2}\times16r$	$4j$; $\frac{p-1}{2}\times8n$ $p\times16r$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Ammm	$C\rightarrow A\rightarrow B$	$a\rightarrow b\rightarrow c\rightarrow a$	$\mathbf{a}\rightarrow\mathbf{b}\rightarrow\mathbf{c}\rightarrow\mathbf{a}$	$x\rightarrow y\rightarrow z\rightarrow x$
Bmmm	$A\rightarrow C\rightarrow B$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 66, pp. 536–537.

$Cccm$ No. 66 $C2/c2/c2/m$ D_{2h}^{20}

	Axes	Coordinates	4a	4b	4c	4d	4e	4f	8g	8h	8i	8j	8k	8l 16m
I Maximal *translationengleiche* subgroups														
[2] $C2cm$ (40) $\widehat{=}$ $Ama2$	 **c**, −**b**, **a**	$x,y,z+\frac{1}{4}$ $z+\frac{1}{4},-y,x$	4a	4a	4b	4b	4b	4b	2×4a	8c	8c	8c	8c	2×4b 2×8c
[2] $Cc2m$ (40) $\widehat{=}$ $Ama2$	 **c**, **a**, **b**	$x,y,z+\frac{1}{4}$ $z+\frac{1}{4},x,y$	4a	4a	4b	4b	4b	4b	8c	2×4a	8c	8c	8c	2×4b 2×8c
[2] $Ccc2$ (37)			4a	4b	4a	4b	4c	4c	8d	8d	2×4a	2×4b	2×4c	8d 2×8d
[2] $C222$ (21)		$x,y,z+\frac{1}{4}$	2a; 2d	2b; 2c	4i	4j	4k	4k	4e; 4f	4g; 4h	2×4i	2×4j	2×4k	8l 2×8l
[2] $C2/c11$ (15) $\widehat{=}$ $C12/c1$	 **b**, **a**, −**c**	 $y,x,-z$	4e	4e	4a	4b	4c	4d	2×4e	8f	8f	8f	8f	8f 2×8f
[2] $C12/c1$ (15)			4e	4e	4a	4b	4c	4d	8f	2×4e	8f	8f	8f	8f 2×8f
[2] $P112/m$ (10)	**a**, $\frac{1}{2}$(−**a**+**b**), **c**	$x+y,2y,z$	2i	2k	1a; 1b	1c; 1f	1e; 1g	1d; 1h	4o	4o	2×2i	2×2k	2j; 2l	2m; 2n 2×4o
	or: $\frac{1}{2}$(**a**−**b**), $\frac{1}{2}$(**a**+**b**), **c**	$x-y,x+y,z$	2i	2l	1a; 1b	1g; 1h	1d; 1f	1c; 1e	4o	4o	2×2i	2×2l	2j; 2k	2m; 2n 2×4o
II Maximal *klassengleiche* subgroups **Loss of centring translations**														
[2] $Pnnm$ (58)			4e	4f	2a; 2b	2c; 2d	4g	4g	8h	8h	2×4e	2×4f	8h	2×4g 2×8h
[2] $Pccn$ (56)		$x+\frac{1}{4},y+\frac{1}{4},z$	4c	4d	4c	4d	4a	4b	8e	8e	2×4c	2×4d	8e	8e 2×8e
[2] $Pcnm$ (53) $\widehat{=}$ $Pmna$	 **c**, −**b**, **a**	$x+\frac{1}{4},y+\frac{1}{4},z$ $z,-y-\frac{1}{4},x+\frac{1}{4}$	4g	4g	4h	4h	2a; 2c	2b; 2d	8i	2×4g	8i	8i	4e; 4f	2×4h 2×8i
[2] $Pncm$ (53) $\widehat{=}$ $Pmna$	 **c**, **a**, **b**	$x+\frac{1}{4},y+\frac{1}{4},z$ $z,x+\frac{1}{4},y+\frac{1}{4}$	4g	4g	4h	4h	2a; 2c	2b; 2d	2×4g	8i	8i	8i	4e; 4f	2×4h 2×8i
[2] $Pncn$ (52) $\widehat{=}$ $Pnna$	 **c**, **a**, **b**	 z,x,y	4c	4c	4a	4b	4d	4d	8e	2×4c	8e	8e	2×4d	8e 2×8e
[2] $Pcnn$ (52) $\widehat{=}$ $Pnna$	 **c**, −**b**, **a**	 $z,-y,x$	4c	4c	4a	4b	4d	4d	2×4c	8e	8e	8e	2×4d	8e 2×8e
[2] $Pccm$ (49)			2e; 2h	2f; 2g	2a; 2b	2c; 2d	4q	4q	4i; 4j	4k; 4l	4m; 4n	4o; 4p	8r	2×4q 2×8r
[2] $Pnnn$ (48)		origin 1: $x,y,z-\frac{1}{4}$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},z$	2a; 2c	2b; 2d	4k	4l	4f	4e	4g; 4h	4i; 4j	2×4k	2×4l	8m	8m 2×8m

	Axes	Coordinates	Wyckoff positions $4a$	$4b$	$4c$	$4d$	$4e$	$4f$ $8j$	$8g$ $8k$	$8h$ $8l$	$8i$ $16m$
Enlarged unit cell, isomorphic											
[3] $Cccm$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a;8g$	$4b;8g$	$4c;8l$	$4d;8l$	$4f;8l$	$4e;8l$ $8j;16m$	$3\times 8g$ $8k;16m$	$8h;16m$ $3\times 8l$	$8i;16m$ $3\times 16m$
[p] $Cccm$	$p\mathbf{a},\mathbf{b},\mathbf{c}$ $p =$ prime > 2; $u = 1,\ldots,p-1$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$4a;$ $\frac{p-1}{2}\times 8g$	$4b;$ $\frac{p-1}{2}\times 8g$	$4c;$ $\frac{p-1}{2}\times 8l$	$4d;$ $\frac{p-1}{2}\times 8l$	$4e;$ $\frac{p-1}{2}\times 8l$	$4f;$ $\frac{p-1}{2}\times 8l$ $8j;$ $\frac{p-1}{2}\times 16m$	$p\times 8g$ $8k;$ $\frac{p-1}{2}\times 16m$	$8h;$ $\frac{p-1}{2}\times 16m$ $p\times 8l$	$8i;$ $\frac{p-1}{2}\times 16m$ $p\times 16m$
[3] $Cccm$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;8h$	$4b;8h$	$4c;8l$	$4d;8l$	$4f;8l$	$4e;8l$ $8j;16m$	$8g;16m$ $8k;16m$	$3\times 8h$ $3\times 8l$	$8i;16m$ $3\times 16m$
[p] $Cccm$	$\mathbf{a},p\mathbf{b},\mathbf{c}$ $p =$ prime > 2; $u = 1,\ldots,p-1$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$4a;$ $\frac{p-1}{2}\times 8h$	$4b;$ $\frac{p-1}{2}\times 8h$	$4c;$ $\frac{p-1}{2}\times 8l$	$4d;$ $\frac{p-1}{2}\times 8l$	$4e;$ $\frac{p-1}{2}\times 8l$	$4f;$ $\frac{p-1}{2}\times 8l$ $8j;$ $\frac{p-1}{2}\times 16m$	$8g;$ $\frac{p-1}{2}\times 16m$ $8k;$ $\frac{p-1}{2}\times 16m$	$p\times 8h$ $p\times 8l$	$8i;$ $\frac{p-1}{2}\times 16m$ $p\times 16m$
[3] $Cccm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$4a;8i$	$4b;8j$	$4c;8i$	$4d;8j$	$4e;8k$	$4f;8k$ $3\times 8j$	$8g;16m$ $3\times 8k$	$8h;16m$ $8l;16m$	$3\times 8i$ $3\times 16m$
[p] $Cccm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p =$ prime > 2; $u = 1,\ldots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$4a;$ $\frac{p-1}{2}\times 8i$	$4b;$ $\frac{p-1}{2}\times 8j$	$4c;$ $\frac{p-1}{2}\times 8i$	$4d;$ $\frac{p-1}{2}\times 8j$	$4e;$ $\frac{p-1}{2}\times 8k$	$4f;$ $\frac{p-1}{2}\times 8k$ $p\times 8j$	$8g;$ $\frac{p-1}{2}\times 16m$ $p\times 8k$	$8h;$ $\frac{p-1}{2}\times 16m$ $8l;$ $\frac{p-1}{2}\times 16m$	$p\times 8i$ $p\times 16m$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Amaa$	$C\to A\to B$	$a\to b\to c\to a$	$\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$	$x\to y\to z\to x$
$Bbmb$	$A\to C\to B$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

Cmme No. 67 $C\,2/m\,2/m\,2/e$ D_{2h}^{21}

	Axes	Coordinates	4*a*	4*b*	4*c*	4*d*	4*e*	4*f*	4*g*	8*h*	8*i*	8*j* 8*m*	8*k* 8*n*	8*l* 16*o*
I Maximal *translationengleiche* subgroups														
[2] *C*2*me* (39) $\hat{=}$ *Aem*2	 **c**, −**b**, **a**	 $z,-y,x$	4*a*	4*b*	4*a*	4*b*	4*c*	4*c*	4*c*	2×4*a*	2×4*b*	8*d* 8*d*	8*d* 2×4*c*	8*d* 2×8*d*
[2] *Cm*2*e* (39) $\hat{=}$ *Aem*2	 **c**, **a**, **b**	$x+\frac{1}{4},y,z$ $z,x+\frac{1}{4},y$	4*a*	4*b*	4*c*	4*c*	4*a*	4*b*	4*c*	8*d*	8*d*	2×4*a* 2×4*c*	2×4*b* 8*d*	8*d* 2×8*d*
[2] *Cmm*2 (35)		$x,y+\frac{1}{4},z$	4*c*	4*c*	4*e*	4*e*	4*d*	4*d*	2*a*; 2*b*	8*f*	8*f*	8*f* 2×4*e*	8*f* 2×4*d*	2×4*c* 2×8*f*
[2] *C*222 (21)		$x+\frac{1}{4},y,z$	2*a*; 2*b*	2*c*; 2*d*	4*e*	4*f*	4*g*	4*h*	4*k*	2×4*e*	2×4*f*	2×4*g* 8*l*	2×4*h* 8*l*	4*i*; 4*j* 2×8*l*
[2] *P*112/*a* (13)	**a**, $\frac{1}{2}$(−**a**+**b**), **c**	$x+y,2y,z$	2*e*	2*e*	2*a*	2*c*	2*d*	2*b*	2*f*	4*g*	4*g*	4*g* 4*g*	4*g* 4*g*	2×2*e* 2×4*g*
[2] *C*2/*m*11 (12) $\hat{=}$ *C*12/*m*1	 **b**, −**a**, **c**	 $y,-x,z$	4*g*	4*h*	2*a*; 2*b*	2*c*; 2*d*	4*e*	4*f*	4*i*	2×4*g*	2×4*h*	8*j* 2×4*i*	8*j* 8*j*	8*j* 2×8*j*
[2] *C*12/*m*1 (12)		$x+\frac{1}{4},y+\frac{1}{4},z$	4*g*	4*h*	4*e*	4*f*	2*a*; 2*b*	2*c*; 2*d*	4*i*	8*j*	8*j*	2×4*g* 8*j*	2×4*h* 2×4*i*	8*j* 2×8*j*
II Maximal *klassengleiche* subgroups														
Loss of centring translations														
[2] *Pmab* (57) $\hat{=}$ *Pbcm*	 **c**, −**b**, **a**	$x+\frac{1}{4},y+\frac{1}{4},z$ $z,-y-\frac{1}{4},x+\frac{1}{4}$	4*c*	4*c*	4*d*	4*d*	4*a*	4*b*	4*d*	8*e*	8*e*	8*e* 2×4*d*	8*e* 8*e*	2×4*c* 2×8*e*
[2] *Pbma* (57) $\hat{=}$ *Pbcm*	 **c**, **a**, **b**	 z,x,y	4*c*	4*c*	4*a*	4*b*	4*d*	4*d*	4*d*	8*e*	8*e*	8*e* 8*e*	8*e* 2×4*d*	2×4*c* 2×8*e*
[2] *Pbaa* (54) $\hat{=}$ *Pcca*	 **b**, **c**, **a**	$x+\frac{1}{4},y+\frac{1}{4},z$ $y+\frac{1}{4},z,x+\frac{1}{4}$	4*d*	4*e*	4*d*	4*e*	4*a*	4*b*	4*c*	2×4*d*	2×4*e*	8*f* 8*f*	8*f* 8*f*	8*f* 2×8*f*
[2] *Pbab* (54) $\hat{=}$ *Pcca*	 **a**, −**c**, **b**	 $x,-z,y$	4*d*	4*e*	4*a*	4*b*	4*d*	4*e*	4*c*	8*f*	8*f*	2×4*d* 8*f*	2×4*e* 8*f*	8*f* 2×8*f*
[2] *Pmma* (51)		$x+\frac{1}{4},y+\frac{1}{4},z$	4*g*	4*h*	4*k*	4*k*	2*a*; 2*b*	2*c*; 2*d*	2*e*; 2*f*	8*l*	8*l*	2×4*g* 2×4*k*	2×4*h* 4*i*; 4*j*	8*l* 2×8*l*
[2] *Pmmb* (51) $\hat{=}$ *Pmma*	 **b**, −**a**, **c**	 $y,-x,z$	4*g*	4*h*	2*a*; 2*b*	2*c*; 2*d*	4*k*	4*k*	2*e*; 2*f*	2×4*g*	2×4*h*	8*l* 4*i*; 4*j*	8*l* 2×4*k*	8*l* 2×8*l*
[2] *Pmaa* (49) $\hat{=}$ *Pccm*	 **b**, **c**, **a**	 y,z,x	2*e*; 2*f*	2*g*; 2*h*	2*a*; 2*d*	2*b*; 2*c*	4*i*	4*j*	4*q*	4*m*; 4*p*	4*n*; 4*o*	2×4*i* 2×4*q*	2×4*j* 8*r*	4*k*; 4*l* 2×8*r*
[2] *Pbmb* (49) $\hat{=}$ *Pccm*	 **c**, **a**, **b**	$x+\frac{1}{4},y+\frac{1}{4},z$ $z,x+\frac{1}{4},y+\frac{1}{4}$	2*e*; 2*g*	2*f*; 2*h*	4*k*	4*l*	2*a*; 2*c*	2*b*; 2*d*	4*q*	2×4*k*	2×4*l*	4*m*; 4*o* 8*r*	4*n*; 4*p* 2×4*q*	4*i*; 4*j* 2×8*r*
Enlarged unit cell, non-isomorphic														
[2] *Imma* (74)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	8*f*	8*g*	4*a*; 4*b*	8*h*	8*i*	4*c*; 4*d*	2×4*e*	2×8*f*	16*j*	16*j* 2×8*h*	2×8*g* 2×8*i*	16*j* 2×16*j*
[2] *Imma* (74)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	8*g*	8*f*	8*h*	4*a*; 4*b*	4*c*; 4*d*	8*i*	2×4*e*	16*j*	2×8*f*	2×8*g* 2×8*h*	16*j* 2×8*i*	16*j* 2×16*j*
[2] *Ibca* (73)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	8*d*	8*c*	8*a*	8*c*	8*d*	8*b*	8*e*	16*f*	2×8*c*	2×8*d* 16*f*	16*f* 16*f*	16*f* 2×16*f*
[2] *Ibca* (73)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	8*c*	8*d*	8*c*	8*a*	8*b*	8*d*	8*e*	2×8*c*	16*f*	16*f* 16*f*	2×8*d* 16*f*	16*f* 2×16*f*
[2] *Imcb* (72) $\hat{=}$ *Ibam*	**a**, **b**, 2**c** **b**, 2**c**, **a**	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$ $y,\frac{1}{2}z,x;+(0,\frac{1}{2},0)$	4*a*; 4*b*	8*g*	4*c*; 4*d*	8*j*	8*f*	8*e*	8*j*	8*h*; 8*i*	16*k*	2×8*f* 2×8*j*	16*k* 16*k*	2×8*g* 2×16*k*

	Axes	Coordinates	Wyckoff positions $4a$	 $4b$ $8i$	 $4c$ $8j$	 $4d$ $8k$	 $4e$ $8l$	 $4f$ $8m$	 $4g$ $8n$	 $8h$ $16o$
[2] $Imcb$ (72) $\widehat{=}$ $Ibam$	**a**, **b**, 2**c** **b**, 2**c**, **a**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ $y,\frac{1}{2}z+\frac{1}{4},x$; $+(0,\frac{1}{2},0)$	$8g$	$4a;4b$ $8h;8i$	$8j$ $16k$	$4c;4d$ $2\times 8f$	$8e$ $2\times 8g$	$8f$ $2\times 8j$	$8j$ $16k$	$16k$ $2\times 16k$
[2] $Icma$ (72) $\widehat{=}$ $Ibam$	**a**, **b**, 2**c** 2**c**, **a**, **b**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z$; $+(0,0,\frac{1}{2})$ $\frac{1}{2}z,x+\frac{1}{4},y+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$4a;4b$	$8f$ $16k$	$8g$ $8h;8i$	$8e$ $16k$	$4c;4d$ $2\times 8f$	$8j$ $16k$	$8j$ $2\times 8j$	$2\times 8g$ $2\times 16k$
[2] $Icma$ (72) $\widehat{=}$ $Ibam$	**a**, **b**, 2**c** 2**c**, **a**, **b**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ $\frac{1}{2}z+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$8f$	$4a;4b$ $2\times 8g$	$8e$ $16k$	$8g$ $8h;8i$	$8j$ $2\times 8f$	$4c;4d$ $16k$	$8j$ $2\times 8j$	$16k$ $2\times 16k$
[2] $Ccce$ (68)	**a**, **b**, 2**c**	origin 1: $x+\frac{1}{4},y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4a;4b$	$8g$ $16i$	$8e$ $2\times 8f$	$8c$ $16i$	$8f$ $2\times 8g$	$8d$ $16i$	$8h$ $16i$	$2\times 8e$ $2\times 16i$
[2] $Ccce$ (68)	**a**, **b**, 2**c**	origin 1: $x+\frac{1}{4},y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$8g$	$4a;4b$ $2\times 8e$	$8c$ $16i$	$8e$ $2\times 8f$	$8d$ $2\times 8g$	$8f$ $16i$	$8h$ $16i$	$16i$ $2\times 16i$
[2] $Cmce$ (64)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$8d$	$8e$ $16g$	$4a;4b$ $16g$	$8f$ $2\times 8e$	$8c$ $16g$	$8e$ $2\times 8f$	$8f$ $16g$	$2\times 8d$ $2\times 16g$
[2] $Cmce$ (64)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$8e$	$8d$ $2\times 8d$	$8f$ $2\times 8e$	$4a;4b$ $16g$	$8e$ $16g$	$8c$ $2\times 8f$	$8f$ $16g$	$16g$ $2\times 16g$
[2] $Ccme$ (64) $\widehat{=}$ $Cmce$	**a**, **b**, 2**c** **b**, −**a**, 2**c**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z$; $+(0,0,\frac{1}{2})$ $y+\frac{1}{4},-x-\frac{1}{4},\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$8d$	$8e$ $2\times 8e$	$8c$ $2\times 8d$	$8e$ $16g$	$4a;4b$ $16g$	$8f$ $16g$	$8f$ $2\times 8f$	$16g$ $2\times 16g$
[2] $Ccme$ (64) $\widehat{=}$ $Cmce$	**a**, **b**, 2**c** **b**, −**a**, 2**c**	$x+\frac{1}{4},y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$ $y+\frac{1}{4},-x-\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$8e$	$8d$ $16g$	$8e$ $16g$	$8c$ $2\times 8d$	$8f$ $16g$	$4a;4b$ $16g$	$8f$ $2\times 8f$	$2\times 8e$ $2\times 16g$
Enlarged unit cell, isomorphic										
[3] $Cmme$	3**a**, **b**, **c**	$\frac{1}{3}x,y,z$; $\pm(\frac{1}{3},0,0)$	$4a;8h$	$4b;8i$ $3\times 8i$	$4c;8h$ $8j;16o$	$4d;8i$ $8k;16o$	$4e;8n$ $8l;16o$	$4f;8n$ $8m;16o$	$4g;8n$ $3\times 8n$	$3\times 8h$ $3\times 16o$
[p] $Cmme$	p**a**, **b**, **c** p = prime > 2; $u=1,\ldots,p-1$	$\frac{1}{p}x,y,z$; $+(\frac{u}{p},0,0)$	$4a$; $\frac{p-1}{2}\times 8h$	$4b$; $\frac{p-1}{2}\times 8i$ $p\times 8i$	$4c$; $\frac{p-1}{2}\times 8h$ $8j$; $\frac{p-1}{2}\times 16o$	$4d$; $\frac{p-1}{2}\times 8i$ $8k$; $\frac{p-1}{2}\times 16o$	$4e$; $\frac{p-1}{2}\times 8n$ $8l$; $\frac{p-1}{2}\times 16o$	$4f$; $\frac{p-1}{2}\times 8n$ $8m$; $\frac{p-1}{2}\times 16o$	$4g$; $\frac{p-1}{2}\times 8n$ $p\times 8n$	$p\times 8h$ $p\times 16o$
[3] $Cmme$	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z$; $\pm(0,\frac{1}{3},0)$	$4a;8j$	$4b;8k$ $8i;16o$	$4c;8m$ $3\times 8j$	$4d;8m$ $3\times 8k$	$4e;8j$ $8l;16o$	$4f;8k$ $3\times 8m$	$4g;8m$ $8n;16o$	$8h;16o$ $3\times 16o$
[p] $Cmme$	**a**, p**b**, **c** p = prime > 2; $u=1,\ldots,p-1$	$x,\frac{1}{p}y,z$; $+(0,\frac{u}{p},0)$	$4a$; $\frac{p-1}{2}\times 8j$	$4b$; $\frac{p-1}{2}\times 8k$ $8i$; $\frac{p-1}{2}\times 16o$	$4c$; $\frac{p-1}{2}\times 8m$ $p\times 8j$	$4d$; $\frac{p-1}{2}\times 8m$ $p\times 8k$	$4e$; $\frac{p-1}{2}\times 8j$ $8l$; $\frac{p-1}{2}\times 16o$	$4f$; $\frac{p-1}{2}\times 8k$ $p\times 8m$	$4g$; $\frac{p-1}{2}\times 8m$ $8n$; $\frac{p-1}{2}\times 16o$	$8h$; $\frac{p-1}{2}\times 16o$ $p\times 16o$
[2] $Cmme$	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a;4b$	$8l$ $16o$	$4c;4d$ $8j;8k$	$8m$ $16o$	$4e;4f$ $2\times 8l$	$8n$ $2\times 8m$	$2\times 4g$ $2\times 8n$	$8h;8i$ $2\times 16o$
[2] $Cmme$	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$8l$	$4a;4b$ $8h;8i$	$8m$ $16o$	$4c;4d$ $8j;8k$	$8n$ $2\times 8l$	$4e;4f$ $2\times 8m$	$2\times 4g$ $2\times 8n$	$16o$ $2\times 16o$
[3] $Cmme$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a;8l$	$4b;8l$ $8i;16o$	$4c;8m$ $8j;16o$	$4d;8m$ $8k;16o$	$4e;8n$ $3\times 8l$	$4f;8n$ $3\times 8m$	$3\times 4g$ $3\times 8n$	$8h;16o$ $3\times 16o$
[p] $Cmme$	**a**, **b**, p**c** p = prime > 2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$4a$; $\frac{p-1}{2}\times 8l$	$4b$; $\frac{p-1}{2}\times 8l$ $p\times 8i$ $\frac{p-1}{2}\times 16o$	$4c$; $\frac{p-1}{2}\times 8m$ $8j$; $\frac{p-1}{2}\times 16o$	$4d$; $\frac{p-1}{2}\times 8m$ $8k$; $\frac{p-1}{2}\times 16o$	$4e$; $\frac{p-1}{2}\times 8n$ $p\times 8l$	$4f$; $\frac{p-1}{2}\times 8n$ $p\times 8m$	$p\times 4g$ $p\times 8n$	$p\times 8h$ $\frac{p-1}{2}\times 16o$ $p\times 16o$

Continued at the bottom of the next page

$Ccce$ No. 68 $C2/c2/c2/e$ D_{2h}^{22}

	Axes	Coordinates origin 1	Coordinates origin 2	4a	4b	8c	8d	8e	8f	8g	8h	16i
I Maximal *translationengleiche* subgroups												
[2] $C2ce$ (41)			$x,y+\frac{1}{4},z+\frac{1}{4}$	4a	4a	8b	8b	2×4a	8b	8b	8b	2×8b
≙ $Aea2$	**c**, −**b**, **a**	$z,-y,x$	$z+\frac{1}{4},-y-\frac{1}{4},x$									
[2] $Cc2e$ (41)			$x,y,z+\frac{1}{4}$	4a	4a	8b	8b	8b	2×4a	8b	8b	2×8b
≙ $Aea2$	**c**, **a**, **b**	z,y,x	$z+\frac{1}{4},x,y$									
[2] $Ccc2$ (37)		$x+\frac{1}{4},y+\frac{1}{4},z$	$x+\frac{1}{4},y,z$	4c	4c	8d	8d	8d	8d	2×4c	4a;4b	2×8d
[2] $C222$ (21)			$x,y+\frac{1}{4},z+\frac{1}{4}$	2a;2c	2b;2d	8l	8l	4e;4f	4g;4h	4i;4j	2×4k	2×8l
[2] $C2/c11$ (15)		$x+\frac{1}{4},y,z+\frac{1}{4}$	$x+\frac{1}{4},y+\frac{1}{4},z$	4e	4e	4a;4b	4c;4d	2×4e	8f	8f	8f	2×8f
≙ $C12/c1$	**b**, −**a**, **c**	$y,-x-\frac{1}{4},z+\frac{1}{4}$	$y+\frac{1}{4},-x-\frac{1}{4},z$									
[2] $C12/c1$ (15)		$x,y+\frac{1}{4},z+\frac{1}{4}$		4e	4e	4c;4d	4a;4b	8f	2×4e	8f	8f	2×8f
[2] $P112/a$ (13)	**a**, $\frac{1}{2}$(−**a**+**b**), **c**	$x+y+\frac{1}{4}$, $2y,z+\frac{1}{4}$	$x+y,2y,z$	2f(e*)	2f(e*)	2b(a*); 2d(c*)	2a(b*); 2c(d*)	4g	4g	2×2f(e*)	2×2e(f*)	2×4g
II Maximal *klassengleiche* subgroups												
Loss of centring translations												
[2] $Pcnb$ (60)		$x,y+\frac{1}{4},z+\frac{1}{4}$		4c	4c	8d	4a;4b	8d	8d	2×4c	8d	2×8d
≙ $Pbcn$	**a**, −**c**, **b**	$x,-z-\frac{1}{4},y+\frac{1}{4}$	$x,-z,y$									
[2] $Pnca$ (60)		$x+\frac{1}{4},y,z+\frac{1}{4}$	$x+\frac{1}{4},y+\frac{1}{4},z$	4c	4c	4a;4b	8d	8d	8d	2×4c	8d	2×8d
≙ $Pbcn$	**b**, **c**, **a**	$y,z+\frac{1}{4},x+\frac{1}{4}$	$y+\frac{1}{4},z,x+\frac{1}{4}$									
[2] $Pcca$ (54)		$x,y+\frac{1}{4},z+\frac{1}{4}$		4c	4c	8f	4a;4b	8f	2×4c	8f	4d;4e	2×8f
[2] $Pccb$ (54)		$x+\frac{1}{4},y,z+\frac{1}{4}$	$x+\frac{1}{4},y+\frac{1}{4},z$	4c	4c	4a;4b	8f	2×4c	8f	8f	4d;4e	2×8f
≙ $Pcca$	**b**, −**a**, **c**	$y,-x-\frac{1}{4},z+\frac{1}{4}$	$y+\frac{1}{4},-x-\frac{1}{4},z$									
[2] $Pnna$ (52)		$x,y+\frac{1}{4},z+\frac{1}{4}$		4d	4d	8e	4a;4b	2×4d	8e	8e	2×4c	2×8e
[2] $Pnnb$ (52)		$x+\frac{1}{4},y,z+\frac{1}{4}$	$x+\frac{1}{4},y+\frac{1}{4},z$	4d	4d	4a;4b	8e	8e	2×4d	8e	2×4c	2×8e
≙ $Pnna$	**b**, −**a**, **c**	$y,-x-\frac{1}{4},z+\frac{1}{4}$	$y+\frac{1}{4},-x-\frac{1}{4},z$									
[2] $Pncb$ (50)				2a;2c	2b;2d	8m	4e;4f	4k;4l	4g;4h	4i;4j	8m	2×8m
≙ $Pban$	**b**, **c**, **a**	y,z,x	y,z,x									
[2] $Pcna$ (50)			$x+\frac{1}{4},y-\frac{1}{4},z$	2a;2c	2b;2d	4e;4f	8m	4i;4j	4k;4l	4g;4h	8m	2×8m
≙ $Pban$	**c**, **a**, **b**	z,x,y	$z,x+\frac{1}{4},y-\frac{1}{4}$									

* origin 2

$Cmme$ No. 67 $C2/m2/m2/e$ CONTINUED (*from preceding page*)

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Aemm$	$C \rightarrow A \rightarrow B$	$a \rightarrow b \rightarrow c \rightarrow a$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$Bmem$	$A \rightarrow C \rightarrow B$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

	Axes	Coordinates origin 1	Coordinates origin 2	4*a*	4*b*	8*c*	8*d*	8*e*	8*f*	8*g*	8*h*	16*i*
Enlarged unit cell, isomorphic												
[3] *Ccce*	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;$ $\pm(\frac{1}{3},0,0)$	$\frac{1}{3}x,y,z;$ $\pm(\frac{1}{3},0,0)$	$4a; 8e$	$4b; 8e$	$8c; 16i$	$8d; 16i$	$3\times 8e$	$8f; 16i$	$8g; 16i$	$8h; 16i$	$3\times 16i$
[*p*] *Ccce*	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;$ $+(\frac{u}{p},0,0)$	$\frac{1}{p}x,y,z;$ $+(\frac{u}{p},0,0)$	$4a;$ $\frac{p-1}{2}\times 8e$	$4b;$ $\frac{p-1}{2}\times 8e$	$8c;$ $\frac{p-1}{2}\times 16i$	$8d;$ $\frac{p-1}{2}\times 16i$	$p\times 8e$	$8f;$ $\frac{p-1}{2}\times 16i$	$8g;$ $\frac{p-1}{2}\times 16i$	$8h;$ $\frac{p-1}{2}\times 16i$	$p\times 16i$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$											
[3] *Ccce*	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;$ $\pm(0,\frac{1}{3},0)$	$x,\frac{1}{3}y,z;$ $\pm(0,\frac{1}{3},0)$	$4a(b^*); 8f$	$4b(a^*); 8f$	$8c; 16i$	$8d; 16i$	$8e; 16i$	$3\times 8f$	$8g; 16i$	$8h; 16i$	$3\times 16i$
[*p*] *Ccce*	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;$ $+(0,\frac{u}{p},0)$	$x,\frac{1}{p}y,z;$ $+(0,\frac{u}{p},0)$	$4a(b^\dagger);$ $\frac{p-1}{2}\times 8f$	$4b(a^\dagger);$ $\frac{p-1}{2}\times 8f$	$8c;$ $\frac{p-1}{2}\times 16i$	$8d;$ $\frac{p-1}{2}\times 16i$	$8e;$ $\frac{p-1}{2}\times 16i$	$p\times 8f$	$8g;$ $\frac{p-1}{2}\times 16i$	$8h;$ $\frac{p-1}{2}\times 16i$	$p\times 16i$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$											
[3] *Ccce*	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$4a(b^*); 8g$	$4b(a^*); 8g$	$8c; 16i$	$8d; 16i$	$8e; 16i$	$8f; 16i$	$3\times 8g$	$3\times 8h$	$3\times 16i$
[*p*] *Ccce*	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$x,y,\frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$4a(b^\dagger);$ $\frac{p-1}{2}\times 8g$	$4b(a^\dagger);$ $\frac{p-1}{2}\times 8g$	$8c;$ $\frac{p-1}{2}\times 16i$	$8d;$ $\frac{p-1}{2}\times 16i$	$8e;$ $\frac{p-1}{2}\times 16i$	$8f;$ $\frac{p-1}{2}\times 16i$	$p\times 8g$	$p\times 8h$	$p\times 16i$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$											

* origin 2
† origin 2 and $p = 4n-1$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$A\,e\,a\,a$	$C \rightarrow A \rightarrow B$	$a \rightarrow b \rightarrow c \rightarrow a$	$\mathbf{a} \rightarrow \mathbf{b} \rightarrow \mathbf{c} \rightarrow \mathbf{a}$	$x \rightarrow y \rightarrow z \rightarrow x$
$B\,b\,e\,b$	$A \rightarrow C \rightarrow B$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

$Fmmm$ No. 69 $F\,2/m\,2/m\,2/m$ D_{2h}^{23}

I Maximal *translationengleiche* subgroups

Subgroup	Axes	Coordinates	$4a$	$4b$	$8c$	$8d$	$8e$	$8f$	$8g$	$8h$	$8i$	$16j$	$16k$ $16n$	$16l$ $16o$	$16m$ $32p$
[2] $F2mm$ (42) $\widehat{=}$ $Fmm2$	 **b**, **c**, **a**	 y,z,x	$4a$	$4a$	$8b$	$8c$	$8d$	$8b$	$2\times4a$	$8d$	$8c$	$16e$	$16e$ $2\times8c$	$2\times8b$ $2\times8d$	$16e$ $2\times16e$
[2] $Fm2m$ (42) $\widehat{=}$ $Fmm2$	 **c**, **a**, **b**	 z,x,y	$4a$	$4a$	$8d$	$8b$	$8c$	$8b$	$8c$	$2\times4a$	$8d$	$16e$	$2\times8b$ $16e$	$16e$ $2\times8c$	$2\times8d$ $2\times16e$
[2] $Fmm2$ (42)			$4a$	$4a$	$8c$	$8d$	$8b$	$8b$	$8d$	$8c$	$2\times4a$	$2\times8b$	$16e$ $2\times8d$	$16e$ $16e$	$2\times8c$ $2\times16e$
[2] $F222$ (22)			$4a$	$4b$	$8j$	$8i$	$8h$	$4c;4d$	$8e$	$8f$	$8g$	$2\times8h$	$2\times8i$ $16k$	$2\times8j$ $16k$	$16k$ $2\times16k$
[2] $B2/m11$ (12) $\widehat{=}$ $C12/m1$	**a**, $\frac{1}{2}$(**b**−**c**), **c** **c**, **a**, $\frac{1}{2}$(**b**−**c**)	$x,2y,y+z$ $y+z,x,2y$	$2a$	$2b$	$2c;2d$	$4e$	$4f$	$4h$	$4g$	$4i$	$4i$	$8j$	$8j$ $8j$	$2\times4h$ $8j$	$2\times4i$ $2\times8j$
[2] $C12/m1$ (12)	**a**, **b**, $\frac{1}{2}$(−**a**+**c**)	$x+z,y,2z$	$2a$	$2b$	$4f$	$2c;2d$	$4e$	$4h$	$4i$	$4g$	$4i$	$8j$	$2\times4h$ $2\times4i$	$8j$ $8j$	$8j$ $2\times8j$
[2] $A112/m$ (12)	$\frac{1}{2}$(**a**−**b**), **b**, **c**	$2x,x+y,z$	$2a$	$2b$	$4e$	$4f$	$2c;2d$	$4h$	$4i$	$4i$	$4g$	$2\times4h$	$8j$ $8j$	$8j$ $2\times4i$	$8j$ $2\times8j$

II Maximal *klassengleiche* subgroups

Loss of centring translations

Subgroup	Axes	Coordinates	$4a$	$4b$	$8c$	$8d$	$8e$	$8f$	$8g$	$8h$	$8i$	$16j$	$16k$ $16n$	$16l$ $16o$	$16m$ $32p$
[2] $Aeaa$ (68) $\widehat{=}$ $Ccce$	 **b**, **c**, **a**	origin 1: x,y,z origin 2: $x+\frac14,y,z+\frac14$ y,z,x (ori. 1) origin 2: $y,z+\frac14,x+\frac14$	$4a$	$4b$	$8h$	$8d$	$8c$	$8h$	$8g$	$8e$	$8f$	$16i$	$16i$ $16i$	$2\times8h$ $16i$	$16i$ $2\times16i$
[2] $Bbeb$ (68) $\widehat{=}$ $Ccce$	 **c**, **a**, **b**	origin 1: x,y,z origin 2: $x+\frac14,y+\frac14,z$ z,x,y (ori. 1) origin 2: $z,x+\frac14,y+\frac14$	$4a$	$4b$	$8c$	$8h$	$8d$	$8h$	$8f$	$8g$	$8e$	$16i$	$2\times8h$ $16i$	$16i$ $16i$	$16i$ $2\times16i$
[2] $Ccce$ (68)		origin 1: x,y,z origin 2: $x,y+\frac14,z+\frac14$	$4a$	$4b$	$8d$	$8c$	$8h$	$8h$	$8e$	$8f$	$8g$	$2\times8h$	$16i$ $16i$	$16i$ $16i$	$16i$ $2\times16i$
[2] $Aemm$ (67) $\widehat{=}$ $Cmme$	 **b**, **c**, **a**	$x+\frac14,y,z+\frac14$ $y,z+\frac14,x+\frac14$	$4g$	$4g$	$8l$	$4c;4d$	$4e;4f$	$4a;4b$	$2\times4g$	$8n$	$8m$	$8j;8k$	$8h;8i$ $2\times8m$	$2\times8l$ $2\times8n$	$16o$ $2\times16o$
[2] $Bmem$ (67) $\widehat{=}$ $Cmme$	 **c**, **a**, **b**	$x+\frac14,y+\frac14,z$ $z,x+\frac14,y+\frac14$	$4g$	$4g$	$4e;4f$	$8l$	$4c;4d$	$4a;4b$	$8m$	$2\times4g$	$8n$	$8h;8i$	$2\times8l$ $16o$	$8j;8k$ $2\times8m$	$2\times8n$ $2\times16o$
[2] $Cmme$ (67)		$x,y+\frac14,z+\frac14$	$4g$	$4g$	$4c;4d$	$4e;4f$	$8l$	$4a;4b$	$8n$	$8m$	$2\times4g$	$2\times8l$	$8j;8k$ $2\times8n$	$8h;8i$ $16o$	$2\times8m$ $2\times16o$
[2] $Amaa$ (66) $\widehat{=}$ $Cccm$	 **b**, **c**, **a**	$x,y+\frac14,z+\frac14$ $y+\frac14,z+\frac14,x$	$4e$	$4f$	$4c;4d$	$8g$	$8h$	$4a;4b$	$8k$	$8l$	$8l$	$2\times8h$	$2\times8g$ $16m$	$8i;8j$ $16m$	$2\times8l$ $2\times16m$
[2] $Bbmb$ (66) $\widehat{=}$ $Cccm$	 **c**, **a**, **b**	$x+\frac14,y,z+\frac14$ $z+\frac14,x+\frac14,y$	$4e$	$4f$	$8h$	$4c;4d$	$8g$	$4a;4b$	$8l$	$8k$	$8l$	$2\times8g$	$8i;8j$ $2\times8l$	$2\times8h$ $16m$	$16m$ $2\times16m$
[2] $Cccm$ (66)		$x+\frac14,y+\frac14,z$	$4e$	$4f$	$8g$	$8h$	$4c;4d$	$4a;4b$	$8l$	$8l$	$8k$	$8i;8j$	$2\times8h$ $16m$	$2\times8g$ $2\times8l$	$16m$ $2\times16m$
[2] $Ammm$ (65) $\widehat{=}$ $Cmmm$	 **b**, **c**, **a**	 y,z,x	$2a;2c$	$2b;2d$	$4e;4f$	$8n$	$8o$	$8m$	$4k;4l$	$4g;4h$	$4i;4j$	$16r$	$16r$ $2\times8n$	$2\times8m$ $2\times8o$	$8p;8q$ $2\times16r$
[2] $Bmmm$ (65) $\widehat{=}$ $Cmmm$	 **c**, **a**, **b**	 z,x,y	$2a;2c$	$2b;2d$	$8o$	$4e;4f$	$8n$	$8m$	$4i;4j$	$4k;4l$	$4g;4h$	$16r$	$2\times8m$ $8p;8q$	$16r$ $2\times8n$	$2\times8o$ $2\times16r$
[2] $Cmmm$ (65)			$2a;2c$	$2b;2d$	$8n$	$8o$	$4e;4f$	$8m$	$4g;4h$	$4i;4j$	$4k;4l$	$2\times8m$	$16r$ $2\times8o$	$16r$ $8p;8q$	$2\times8n$ $2\times16r$

	Axes	Coordinates	Wyckoff positions									
			$4a$	$4b$	$8c$	$8d$	$8e$ $16k$	$8f$ $16l$	$8g$ $16m$	$8h$ $16n$	$8i$ $16o$	$16j$ $32p$
[2] *Aema* (64) $\widehat{=}$ *Cmce*	**b**, **c**, **a**	y,z,x	$4a$	$4b$	$8c$	$8f$	$8e$ $16g$	$8e$ $16g$	$8f$ $16g$	$8d$ $2\times 8f$	$8f$ $16g$	$2\times 8e$ $2\times 16g$
[2] *Aeam* (64) $\widehat{=}$ *Cmce*	**c**, −**b**, **a**	$z,-y,x$	$4a$	$4b$	$8c$	$8e$	$8f$ $2\times 8e$	$8e$ $16g$	$8f$ $16g$	$8f$ $16g$	$8d$ $2\times 8f$	$16g$ $2\times 16g$
[2] *Bbem* (64) $\widehat{=}$ *Cmce*	**c**, **a**, **b**	z,x,y	$4a$	$4b$	$8e$	$8c$	$8f$ $16g$	$8e$ $2\times 8e$	$8f$ $16g$	$8f$ $16g$	$8d$ $2\times 8f$	$16g$ $2\times 16g$
[2] *Bmeb* (64) $\widehat{=}$ *Cmce*	**a**, −**c**, **b**	$x,-z,y$	$4a$	$4b$	$8f$	$8c$	$8e$ $16g$	$8e$ $16g$	$8d$ $2\times 8f$	$8f$ $16g$	$8f$ $16g$	$2\times 8e$ $2\times 16g$
[2] *Cmce* (64)			$4a$	$4b$	$8f$	$8e$	$8c$ $2\times 8e$	$8e$ $16g$	$8d$ $2\times 8f$	$8f$ $16g$	$8f$ $16g$	$16g$ $2\times 16g$
[2] *Ccme* (64) $\widehat{=}$ *Cmce*	**b**, −**a**, **c**	$y,-x,z$	$4a$	$4b$	$8e$	$8f$	$8c$ $16g$	$8e$ $2\times 8e$	$8f$ $16g$	$8d$ $2\times 8f$	$8f$ $16g$	$16g$ $2\times 16g$
[2] *Amam* (63) $\widehat{=}$ *Cmcm*	**c**, −**b**, **a**	$x+\frac{1}{4},y+\frac{1}{4},z$ $z,-y-\frac{1}{4},x+\frac{1}{4}$	$4c$	$4c$	$8g$	$8d$	$4a;4b$ $16h$	$8e$ $16h$	$8f$ $2\times 8g$	$2\times 4c$ $16h$	$8g$ $2\times 8f$	$2\times 8e$ $2\times 16h$
[2] *Amma* (63) $\widehat{=}$ *Cmcm*	**b**, **c**, **a**	$x+\frac{1}{4},y,z+\frac{1}{4}$ $y,z+\frac{1}{4},x+\frac{1}{4}$	$4c$	$4c$	$8g$	$4a;4b$	$8d$ $2\times 8e$	$8e$ $16h$	$8f$ $2\times 8g$	$8g$ $2\times 8f$	$2\times 4c$ $16h$	$16h$ $2\times 16h$
[2] *Bbmm* (63) $\widehat{=}$ *Cmcm*	**c**, **a**, **b**	$x+\frac{1}{4},y+\frac{1}{4},z$ $z,x+\frac{1}{4},y+\frac{1}{4}$	$4c$	$4c$	$8d$	$8g$	$4a;4b$ $16h$	$8e$ $16h$	$2\times 4c$ $16h$	$8f$ $2\times 8g$	$8g$ $2\times 8f$	$2\times 8e$ $2\times 16h$
[2] *Bmmb* (63) $\widehat{=}$ *Cmcm*	**a**, −**c**, **b**	$x,y+\frac{1}{4},z+\frac{1}{4}$ $x,-z-\frac{1}{4},y+\frac{1}{4}$	$4c$	$4c$	$4a;4b$	$8g$	$8d$ $16h$	$8e$ $2\times 8e$	$8g$ $2\times 8f$	$8f$ $2\times 8g$	$2\times 4c$ $16h$	$16h$ $2\times 16h$
[2] *Ccmm* (63) $\widehat{=}$ *Cmcm*	**b**, −**a**, **c**	$x+\frac{1}{4},y,z+\frac{1}{4}$ $y,-x-\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$8d$	$4a;4b$	$8g$ $2\times 8e$	$8e$ $16h$	$2\times 4c$ $16h$	$8g$ $2\times 8f$	$8f$ $2\times 8g$	$16h$ $2\times 16h$
[2] *Cmcm* (63)		$x,y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$4a;4b$	$8d$	$8g$ $16h$	$8e$ $2\times 8e$	$8g$ $2\times 8f$	$2\times 4c$ $16h$	$8f$ $2\times 8g$	$16h$ $2\times 16h$
Enlarged unit cell, isomorphic												
[3] *Fmmm*	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;$ $\pm(\frac{1}{3},0,0)$	$4a;8g$	$4b;8g$	$8c;16l$	$8d;16n$	$8e;16o$ $16k;32p$	$8f;16l$ $3\times 16l$	$3\times 8g$ $16m;32p$	$8h;16o$ $3\times 16n$	$8i;16n$ $3\times 16o$	$16j;32p$ $3\times 32p$
[p] *Fmmm*	p**a**, **b**, **c** $p=$ prime >2; $u=1,\dots,p-1$	$\frac{1}{p}x,y,z;$ $+(\frac{u}{p},0,0)$	$4a;$ $\frac{p-1}{2}\times 8g$	$4b;$ $\frac{p-1}{2}\times 8g$	$8c;$ $\frac{p-1}{2}\times 16l$	$8d;$ $\frac{p-1}{2}\times 16n$	$8e;$ $\frac{p-1}{2}\times 16o$ $16k;$ $\frac{p-1}{2}\times 32p$	$8f;$ $\frac{p-1}{2}\times 16l$ $p\times 16l$	$p\times 8g$ $16m;$ $\frac{p-1}{2}\times 32p$	$8h;$ $\frac{p-1}{2}\times 16o$ $p\times 16n$	$8i;$ $\frac{p-1}{2}\times 16n$ $p\times 16o$	$16j;$ $\frac{p-1}{2}\times 32p$ $p\times 32p$
[3] *Fmmm*	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;$ $\pm(0,\frac{1}{3},0)$	$4a;8h$	$4b;8h$	$8c;16m$	$8d;16k$	$8e;16o$ $3\times 16k$	$8f;16k$ $16l;32p$	$8g;16o$ $3\times 16m$	$3\times 8h$ $16n;32p$	$8i;16m$ $3\times 16o$	$16j;32p$ $3\times 32p$
[p] *Fmmm*	**a**, p**b**, **c** $p=$ prime >2; $u=1,\dots,p-1$	$x,\frac{1}{p}y,z;$ $+(0,\frac{u}{p},0)$	$4a;$ $\frac{p-1}{2}\times 8h$	$4b;$ $\frac{p-1}{2}\times 8h$	$8c;$ $\frac{p-1}{2}\times 16m$	$8d;$ $\frac{p-1}{2}\times 16k$	$8e;$ $\frac{p-1}{2}\times 16o$ $p\times 16k$	$8f;$ $\frac{p-1}{2}\times 16k$ $16l;$ $\frac{p-1}{2}\times 32p$	$8g;$ $\frac{p-1}{2}\times 16o$ $p\times 16m$	$p\times 8h$ $16n;$ $\frac{p-1}{2}\times 32p$	$8i;$ $\frac{p-1}{2}\times 16m$ $p\times 16o$	$16j;$ $\frac{p-1}{2}\times 32p$ $p\times 32p$
[3] *Fmmm*	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$4a;8i$	$4b;8i$	$8c;16m$	$8d;16n$	$8e;16j$ $16k;32p$	$8f;16j$ $16l;32p$	$8g;16n$ $3\times 16m$	$8h;16m$ $3\times 16n$	$3\times 8i$ $16o;32p$	$3\times 16j$ $3\times 32p$
[p] *Fmmm*	**a**, **b**, p**c** $p=$ prime >2; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$4a;$ $\frac{p-1}{2}\times 8i$	$4b;$ $\frac{p-1}{2}\times 8i$	$8c;$ $\frac{p-1}{2}\times 16m$	$8d;$ $\frac{p-1}{2}\times 16n$	$8e;$ $\frac{p-1}{2}\times 16j$ $16k;$ $\frac{p-1}{2}\times 32p$	$8f;$ $\frac{p-1}{2}\times 16j$ $16l;$ $\frac{p-1}{2}\times 32p$	$8g;$ $\frac{p-1}{2}\times 16n$ $p\times 16m$	$8h;$ $\frac{p-1}{2}\times 16m$ $p\times 16n$	$p\times 8i$ $16o;$ $\frac{p-1}{2}\times 32p$	$p\times 16j$ $p\times 32p$

$F\,d\,d\,d$ No. 70 $F\,2/d\,2/d\,2/d$ D_{2h}^{24}

I Maximal *translationengleiche* subgroups

Subgroup	Axes	Coordinates: origin 1	Coordinates: origin 2	$8a$	$8b$	$16c$	$16d$	$16e$	$16f$	$16g$	$32h$
[2] $F2dd$ (43)			$x, y+\frac{1}{8}, z+\frac{1}{8}$	$8a$	$8a$	$16b$	$16b$	$2\times 8a$	$16b$	$16b$	$2\times 16b$
$\widehat{=}\,Fdd2$	**b**, **c**, **a**	y, z, x	$y+\frac{1}{8}, z+\frac{1}{8}, x$								
[2] $Fd2d$ (43)			$x+\frac{1}{8}, y, z+\frac{1}{8}$	$8a$	$8a$	$16b$	$16b$	$16b$	$2\times 8a$	$16b$	$2\times 16b$
$\widehat{=}\,Fdd2$	**c**, **a**, **b**	z, x, y	$z+\frac{1}{8}, x+\frac{1}{8}, y$								
[2] $Fdd2$ (43)			$x+\frac{1}{8}, y+\frac{1}{8}, z$	$8a$	$8a$	$16b$	$16b$	$16b$	$16b$	$2\times 8a$	$2\times 16b$
[2] $F222$ (22)			$x+\frac{1}{8}, y+\frac{1}{8}, z+\frac{1}{8}$	$4a; 4c$	$4b; 4d$	$16k$	$16k$	$8e; 8j$	$8f; 8i$	$8g; 8h$	$2\times 16k$
[2] $C2/c11$ (15)	$-$**a**, **b**, $-\frac{1}{2}$(**b**+**c**)	$-x+\frac{1}{8}, y-z, -2z+\frac{1}{4}$	$-x, y-z, -2z$	$4e$	$4e$	$4a; 4c$	$4b; 4d$	$2\times 4e$	$8f$	$8f$	$2\times 8f$
$\widehat{=}\,C12/c1$	**b**, **a**, $-\frac{1}{2}$(**b**+**c**)	$y-z, x-\frac{1}{8}, -2z+\frac{1}{4}$	$y-z, x, -2z$								
[2] $C12/c1$ (15)	**a**, $-$**b**, $-\frac{1}{2}$(**a**+**c**)	$x-z, -y+\frac{1}{8}, -2z+\frac{1}{4}$	$x-z, -y, -2z$	$4e$	$4e$	$4a; 4d$	$4b; 4c$	$8f$	$2\times 4e$	$8f$	$2\times 8f$
[2] $A112/a$ (15)	$-\frac{1}{2}$(**a**+**b**), **b**, $-$**c**	$-2x+\frac{1}{4}, -x+y, -z+\frac{1}{8}$	$-2x, -x+y, -z$	$4e$	$4e$	$4a; 4d$	$4b; 4c$	$8f$	$8f$	$2\times 4e$	$2\times 8f$

Enlarged unit cell, isomorphic

Subgroup	Axes	origin 1	origin 2	$8a$	$8b$	$16c$	$16d$	$16e$	$16f$	$16g$	$32h$
[3] $Fddd$	3**a**, **b**, **c**	$\frac{1}{3}x-\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$; $\pm(\frac{1}{3}, 0, 0)$	$\frac{1}{3}x, y+\frac{1}{4}, z+\frac{1}{4}$; $\pm(\frac{1}{3}, 0, 0)$	$8b; 16e$	$8a; 16e$	$16c; 32h$	$16d; 32h$	$3\times 16e$	$16f; 32h$	$16g; 32h$	$3\times 32h$
[p] $Fddd$	p**a**, **b**, **c** p = prime = $4n+1$; $u = 1, \ldots, p-1$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$\frac{1}{p}x, y, z; +(\frac{u}{p}, 0, 0)$	$8a(b^*)$; $\frac{p-1}{2}\times 16e$	$8b(a^*)$; $\frac{p-1}{2}\times 16e$	$16c(d^\dagger)$; $\frac{p-1}{2}\times 32h$	$16d(c^\dagger)$; $\frac{p-1}{2}\times 32h$	$p\times 16e$	$16f$; $\frac{p-1}{2}\times 32h$	$16g$; $\frac{p-1}{2}\times 32h$	$p\times 32h$
[p] $Fddd$	p**a**, **b**, **c** p = prime = $4n-1$; $u = 1, \ldots, p-1$	$\frac{1}{p}x-\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$; $+(\frac{u}{p}, 0, 0)$	$\frac{1}{p}x, y+\frac{1}{4}, z+\frac{1}{4}$; $+(\frac{u}{p}, 0, 0)$	$8b(a^\ddagger)$; $\frac{p-1}{2}\times 16e$	$8a(b^\ddagger)$; $\frac{p-1}{2}\times 16e$	$16c(d^\S)$; $\frac{p-1}{2}\times 32h$	$16d(c^\S)$; $\frac{p-1}{2}\times 32h$	$p\times 16e$	$16f$; $\frac{p-1}{2}\times 32h$	$16g$; $\frac{p-1}{2}\times 32h$	$p\times 32h$
[3] $Fddd$	**a**, 3**b**, **c**	$x+\frac{1}{4}, \frac{1}{3}y-\frac{1}{4}, z+\frac{1}{4}$; $\pm(0, \frac{1}{3}, 0)$	$x+\frac{1}{4}, \frac{1}{3}y, z+\frac{1}{4}$; $\pm(0, \frac{1}{3}, 0)$	$8b; 16f$	$8a; 16f$	$16c; 32h$	$16d; 32h$	$16e; 32h$	$3\times 16f$	$16g; 32h$	$3\times 32h$
[p] $Fddd$	**a**, p**b**, **c** p = prime = $4n+1$; $u = 1, \ldots, p-1$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$x, \frac{1}{p}y, z; +(0, \frac{u}{p}, 0)$	$8a(b^*)$; $\frac{p-1}{2}\times 16f$	$8b(a^*)$; $\frac{p-1}{2}\times 16f$	$16c(d^\dagger)$; $\frac{p-1}{2}\times 32h$	$16d(c^\dagger)$; $\frac{p-1}{2}\times 32h$	$16e$; $\frac{p-1}{2}\times 32h$	$p\times 16f$	$16g$; $\frac{p-1}{2}\times 32h$	$p\times 32h$
[p] $Fddd$	**a**, p**b**, **c** p = prime = $4n-1$; $u = 1, \ldots, p-1$	$x+\frac{1}{4}, \frac{1}{p}y-\frac{1}{4}, z+\frac{1}{4}$; $+(0, \frac{u}{p}, 0)$	$x+\frac{1}{4}, \frac{1}{p}y, z+\frac{1}{4}$; $+(0, \frac{u}{p}, 0)$	$8b(a^\ddagger)$; $\frac{p-1}{2}\times 16f$	$8a(b^\ddagger)$; $\frac{p-1}{2}\times 16f$	$16c(d^\S)$; $\frac{p-1}{2}\times 32h$	$16d(c^\S)$; $\frac{p-1}{2}\times 32h$	$16e$; $\frac{p-1}{2}\times 32h$	$p\times 16f$	$16g$; $\frac{p-1}{2}\times 32h$	$p\times 32h$
[3] $Fddd$	**a**, **b**, 3**c**	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{3}z-\frac{1}{4}$; $\pm(0, 0, \frac{1}{3})$	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$8b; 16g$	$8a; 16g$	$16c; 32h$	$16d; 32h$	$16e; 32h$	$16f; 32h$	$3\times 16g$	$3\times 32h$
[p] $Fddd$	**a**, **b**, p**c** p = prime = $4n+1$; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$8a(b^*)$; $\frac{p-1}{2}\times 16g$	$8b(a^*)$; $\frac{p-1}{2}\times 16g$	$16c(d^\dagger)$; $\frac{p-1}{2}\times 32h$	$16d(c^\dagger)$; $\frac{p-1}{2}\times 32h$	$16e$ $\frac{p-1}{2}\times 32h$	$16f$; $\frac{p-1}{2}\times 32h$	$p\times 16g$	$p\times 32h$
[p] $Fddd$	**a**, **b**, p**c** p = prime = $4n-1$; $u = 1, \ldots, p-1$	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{p}z-\frac{1}{4}$; $+(\frac{u}{p}, 0, 0)$	$x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{p}z$; $+(\frac{u}{p}, 0, 0)$	$8b(a^\ddagger)$; $\frac{p-1}{2}\times 16g$	$8a(b^\ddagger)$; $\frac{p-1}{2}\times 16g$	$16c(d^\S)$; $\frac{p-1}{2}\times 32h$	$16d(c^\S)$; $\frac{p-1}{2}\times 32h$	$16e$; $\frac{p-1}{2}\times 32h$	$16f$; $\frac{p-1}{2}\times 32h$	$p\times 16g$	$p\times 32h$

* origin 2 and $p = 8n+5$
† origin 1 and $p = 8n+5$
‡ origin 2 and $p = 8n+7$
§ origin 1 and $p = 8n+7$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 71, pp. 545–546.

D_{2h}^{25} $\quad I\,2/m\,2/m\,2/m$ $\quad$ No. 71 $\quad$ $I\,m\,m\,m$

	Axes	Coordinates	Wyckoff positions											
			$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$4i$	$4j$ $8m$	$8k$ $8n$	$8l$ $16o$
I Maximal *translationengleiche* subgroups														
[2] $I2mm$ (44) ≙ $Imm2$	**b**, **c**, **a**	y,z,x	$2a$	$2a$	$2b$	$2b$	$2{\times}2a$	$2{\times}2b$	$4c$	$4c$	$4d$	$4d$ $2{\times}4d$	$8e$ $2{\times}4c$	$8e$ $2{\times}8e$
[2] $Im2m$ (44) ≙ $Imm2$	**c**, **a**, **b**	z,x,y	$2a$	$2b$	$2b$	$2a$	$4d$	$4d$	$2{\times}2a$	$2{\times}2b$	$4c$	$4c$ $8e$	$8e$ $2{\times}4d$	$2{\times}4c$ $2{\times}8e$
[2] $Imm2$ (44)			$2a$	$2b$	$2a$	$2b$	$4c$	$4c$	$4d$	$4d$	$2{\times}2a$	$2{\times}2b$ $2{\times}4c$	$8e$ $8e$	$2{\times}4d$ $2{\times}8e$
[2] $I222$ (23)			$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$4i$	$4j$ $8k$	$8k$ $8k$	$8k$ $2{\times}8k$
[2] $I2/m11$ (12) ≙ $I12/m1$ ≙ $C12/m1$	 **c**, **a**, **b** **−b−c**, **a**, **c**	 z,x,y $-y,x,-y+z$	$2a$	$2b$	$2c$	$2d$	$4g$	$4h$	$4i$	$4i$	$4i$	$4i$ $8j$	$4e;4f$ $8j$	$2{\times}4i$ $2{\times}8j$
[2] $I12/m1$ (12) ≙ $C12/m1$	 **−a−c**, **b**, **a**	 $-z,y,x-z$	$2a$	$2c$	$2d$	$2b$	$4i$	$4i$	$4g$	$4h$	$4i$	$4i$ $2{\times}4i$	$4e;4f$ $8j$	$8j$ $2{\times}8j$
[2] $I112/m$ (12) ≙ $A112/m$	 **b**, **−a−b**, **c**	 $-x+y,-x,z$	$2a$	$2d$	$2b$	$2c$	$4i$	$4i$	$4i$	$4i$	$4g$	$4h$ $8j$	$4e;4f$ $2{\times}4i$	$8j$ $2{\times}8j$
II Maximal *klassengleiche* subgroups **Loss of centring translations**														
[2] $Pmmn$ (59)		origin 1: $x,y,z+\frac{1}{4}$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$2a$	$2b$	$2a$	$2b$	$4f$	$4f$	$4e$	$4e$	$2{\times}2a$	$2{\times}2b$ $2{\times}4f$	$4c;4d$ $8g$	$2{\times}4e$ $2{\times}8g$
[2] $Pmnm$ (59) ≙ $Pmmn$	 **c**, **a**, **b**	origin 1: $x,y+\frac{1}{4},z$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$ $z,x,y+\frac{1}{4}$ (origin 1) $z+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$ (origin 2)	$2a$	$2b$	$2b$	$2a$	$4e$	$4e$	$2{\times}2a$	$2{\times}2b$	$4f$	$4f$ $8g$	$4c;4d$ $2{\times}4e$	$2{\times}4f$ $2{\times}8g$
[2] $Pnmm$ (59) ≙ $Pmmn$	 **b**, **c**, **a**	origin 1: $x+\frac{1}{4},y,z$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$ $y,z,x+\frac{1}{4}$ (origin 1) $y+\frac{1}{4},z+\frac{1}{4},x+\frac{1}{4}$ (origin 2)	$2a$	$2a$	$2b$	$2b$	$2{\times}2a$	$2{\times}2b$	$4f$	$4f$	$4e$	$4e$ $2{\times}4e$	$4c;4d$ $2{\times}4f$	$8g$ $2{\times}8g$
[2] $Pnnm$ (58)			$2a$	$2d$	$2b$	$2c$	$4g$	$4g$	$4g$	$4g$	$4e$	$4f$ $8h$	$8h$ $2{\times}4g$	$8h$ $2{\times}8h$
[2] $Pnmn$ (58) ≙ $Pnnm$	 **c**, **a**, **b**	 z,x,y	$2a$	$2c$	$2d$	$2b$	$4g$	$4g$	$4e$	$4f$	$4g$	$4g$ $2{\times}4g$	$8h$ $8h$	$8h$ $2{\times}8h$
[2] $Pmnn$ (58) ≙ $Pnnm$	 **b**, **c**, **a**	 y,z,x	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4g$	$4g$	$4g$ $8h$	$8h$ $8h$	$2{\times}4g$ $2{\times}8h$
[2] $Pnnn$ (48)		origin 1: x,y,z origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$2a$	$2b$	$2c$	$2d$	$4g$	$4h$	$4i$	$4j$	$4k$	$4l$ $8m$	$4e;4f$ $8m$	$8m$ $2{\times}8m$
[2] $Pmmm$ (47)			$1a;1h$	$1b;1g$	$1c;1f$	$1d;1e$	$2i;2l$	$2j;2k$	$2m;2p$	$2n;2o$	$2q;2t$	$2r;2s$ $4w;4x$	8α $4y;4z$	$4u;4v$ $2{\times}8\alpha$

	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$ / $8k$	$4g$ / $8l$	$4h$ / $8m$	$4i$ / $8n$	$4j$ / $16o$
Enlarged unit cell, isomorphic												
[3] *Immm*	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$2a;4e$	$2b;4e$	$2c;4f$	$2d;4f$	$3\times4e$	$3\times4f$	$4g;8n$	$4h;8n$	$4i;8m$	$4j;8m$
								$8k;16o$	$8l;16o$	$3\times8m$	$3\times8n$	$3\times16o$
[p] *Immm*	p**a**, **b**, **c**	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$ p = prime >2; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}\times4e$	$2b;$ $\frac{p-1}{2}\times4e$	$2c;$ $\frac{p-1}{2}\times4f$	$2d;$ $\frac{p-1}{2}\times4f$	$p\times4e$	$p\times4f$	$4g;$ $\frac{p-1}{2}\times8n$	$4h;$ $\frac{p-1}{2}\times8n$	$4i;$ $\frac{p-1}{2}\times8m$	$4j;$ $\frac{p-1}{2}\times8m$
								$8k;$ $\frac{p-1}{2}\times16o$	$8l;$ $\frac{p-1}{2}\times16o$	$p\times8m$	$p\times8n$	$p\times16o$
[3] *Immm*	**a**,3**b**,**c**	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$2a;4g$	$2b;4h$	$2c;4h$	$2d;4g$	$4e;8n$	$4f;8n$	$3\times4g$	$3\times4h$	$4i;8l$	$4j;8l$
								$8k;16o$	$3\times8l$	$8m;16o$	$3\times8n$	$3\times16o$
[p] *Immm*	**a**,p**b**,**c**	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$ p = prime >2; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}\times4g$	$2b;$ $\frac{p-1}{2}\times4h$	$2c;$ $\frac{p-1}{2}\times4h$	$2d;$ $\frac{p-1}{2}\times4g$	$4e;$ $\frac{p-1}{2}\times8n$	$4f;$ $\frac{p-1}{2}\times8n$	$p\times4g$	$p\times4h$	$4i;$ $\frac{p-1}{2}\times8l$	$4j;$ $\frac{p-1}{2}\times8l$
								$8k;$ $\frac{p-1}{2}\times16o$	$p\times8l$	$8m;$ $\frac{p-1}{2}\times16o$	$p\times8n$	$p\times16o$
[3] *Immm*	**a**,**b**,3**c**	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4i$	$2b;4j$	$2c;4i$	$2d;4j$	$4e;8m$	$4f;8m$	$4g;8l$	$4h;8l$	$3\times4i$	$3\times4j$
								$8k;16o$	$3\times8l$	$3\times8m$	$8n;16o$	$3\times16o$
[p] *Immm*	**a**,**b**,p**c**	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ p = prime >2; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}\times4i$	$2b;$ $\frac{p-1}{2}\times4j$	$2c;$ $\frac{p-1}{2}\times4i$	$2d;$ $\frac{p-1}{2}\times4j$	$4e;$ $\frac{p-1}{2}\times8m$	$4f;$ $\frac{p-1}{2}\times8m$	$4g;$ $\frac{p-1}{2}\times8l$	$4h;$ $\frac{p-1}{2}\times8l$	$p\times4i$	$p\times4j$
								$8k;$ $\frac{p-1}{2}\times16o$	$p\times8l$	$p\times8m$	$8n;$ $\frac{p-1}{2}\times16o$	$p\times16o$

D_{2h}^{26} $I\,2/b\,2/a\,2/m$ No. 72 $I\,b\,a\,m$

	Axes	Coordinates	Wyckoff positions										
			$4a$	$4b$	$4c$	$4d$	$8e$	$8f$	$8g$	$8h$	$8i$	$8j$	$16k$
I Maximal *translationengleiche* subgroups													
[2] $I2cm$ (46)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4b$	$4b$	$8c$	$2\times4a$	$8c$	$8c$	$8c$	$2\times4b$	$2\times8c$
$\widehat{=}$ $Ima2$	$\mathbf{c}, -\mathbf{b}, \mathbf{a}$	$z+\frac{1}{4},-y,x$											
[2] $Ic2m$ (46)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4b$	$4b$	$8c$	$8c$	$2\times4a$	$8c$	$8c$	$2\times4b$	$2\times8c$
$\widehat{=}$ $Ima2$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z+\frac{1}{4},x,y$											
[2] $Iba2$ (45)			$4a$	$4b$	$4a$	$4b$	$8c$	$8c$	$8c$	$2\times4a$	$2\times4b$	$8c$	$2\times8c$
[2] $I222$ (23)		$x,y,z+\frac{1}{4}$	$2a;2c$	$2b;2d$	$4i$	$4j$	$8k$	$4e;4f$	$4g;4h$	$2\times4i$	$2\times4j$	$8k$	$2\times8k$
[2] $I2/c11$ (15)			$4e$	$4e$	$4a$	$4b$	$4c;4d$	$2\times4e$	$8f$	$8f$	$8f$	$8f$	$2\times8f$
$\widehat{=}$ $I12/a1$	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z,x,y											
$\widehat{=}$ $C12/c1$	$-\mathbf{b}-\mathbf{c}, \mathbf{a}, \mathbf{c}$	$-y,x,-y+z$											
[2] $I12/c1$ (15)			$4e$	$4e$	$4a$	$4b$	$4c;4d$	$8f$	$2\times4e$	$8f$	$8f$	$8f$	$2\times8f$
$\widehat{=}$ $C12/c1$	$\mathbf{a}-\mathbf{c}, \mathbf{b}, \mathbf{c}$	$x,y,x+z$											
[2] $I112/m$ (12)			$4g$	$4h$	$2a;2b$	$2c;2d$	$4e;4f$	$8j$	$8j$	$2\times4g$	$2\times4h$	$2\times4i$	$2\times8j$
$\widehat{=}$ $A112/m$	$\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-x+y,-y,z$											
II Maximal *klassengleiche* subgroups													
Loss of centring translations													
[2] $Pbcn$ (60)			$4c$	$4c$	$4a$	$4b$	$8d$	$8d$	$2\times4c$	$8d$	$8d$	$8d$	$2\times8d$
[2] $Pcan$ (60)			$4c$	$4c$	$4a$	$4b$	$8d$	$2\times4c$	$8d$	$8d$	$8d$	$8d$	$2\times8d$
$\widehat{=}$ $Pbcn$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y,-x,z$											
[2] $Pbcm$ (57)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$4d$	$4d$	$4a;4b$	$2\times4c$	$8e$	$8e$	$8e$	$2\times4d$	$2\times8e$
[2] $Pcam$ (57)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$4d$	$4d$	$4a;4b$	$8e$	$2\times4c$	$8e$	$8e$	$2\times4d$	$2\times8e$
$\widehat{=}$ $Pbcm$	$\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$y+\frac{1}{4},-x-\frac{1}{4},z+\frac{1}{4}$											
[2] $Pccn$ (56)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4d$	$4c$	$4d$	$4a;4b$	$8e$	$8e$	$2\times4c$	$2\times4d$	$8e$	$2\times8e$
[2] $Pbam$ (55)			$4e$	$4f$	$2a;2b$	$2c;2d$	$8i$	$8i$	$8i$	$2\times4e$	$2\times4f$	$4g;4h$	$2\times8i$
[2] $Pban$ (50)	origin 1:	$x,y,z+\frac{1}{4}$	$2a;2d$	$2b;2c$	$4k$	$4l$	$4e;4f$	$4g;4h$	$4i;4j$	$2\times4k$	$2\times4l$	$8m$	$2\times8m$
	origin 2:	$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$											
[2] $Pccm$ (49)			$2e;2h$	$2f;2g$	$2a;2b$	$2c;2d$	$8r$	$4i;4j$	$4k;4l$	$4m;4n$	$4o;4p$	$2\times4q$	$2\times8r$
Enlarged unit cell, isomorphic													
[3] $Ibam$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{3}x,y,z;\pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4c;8j$	$4d;8j$	$8e;16k$	$3\times8f$	$8g;16k$	$8h;16k$	$8i;16k$	$3\times8j$	$3\times16k$
[p] $Ibam$	$p\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{p}x,y,z;+(\frac{u}{p},0,0)$	$4a;$ $\frac{p-1}{2}\times 8f$	$4b;$ $\frac{p-1}{2}\times 8f$	$4c;$ $\frac{p-1}{2}\times 8j$	$4d;$ $\frac{p-1}{2}\times 8j$	$8e;$ $\frac{p-1}{2}\times 16k$	$p\times8f$	$8g;$ $\frac{p-1}{2}\times 16k$	$8h;$ $\frac{p-1}{2}\times 16k$	$8i;$ $\frac{p-1}{2}\times 16k$	$p\times8j$	$p\times16k$
	p = prime > 2; $u = 1,\ldots,p-1$												
[3] $Ibam$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$x,\frac{1}{3}y,z;\pm(0,\frac{1}{3},0)$	$4a;8g$	$4b;8g$	$4c;8j$	$4d;8j$	$8e;16k$	$8f;16k$	$3\times8g$	$8h;16k$	$8i;16k$	$3\times8j$	$3\times16k$
[p] $Ibam$	$\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$x,\frac{1}{p}y,z;+(0,\frac{u}{p},0)$	$4a;$ $\frac{p-1}{2}\times 8g$	$4b;$ $\frac{p-1}{2}\times 8g$	$4c;$ $\frac{p-1}{2}\times 8j$	$4d;$ $\frac{p-1}{2}\times 8j$	$8e;$ $\frac{p-1}{2}\times 16k$	$8f;$ $\frac{p-1}{2}\times 16k$	$p\times8g$	$8h;$ $\frac{p-1}{2}\times 16k$	$8i;$ $\frac{p-1}{2}\times 16k$	$p\times8j$	$p\times16k$
	p = prime > 2; $u = 1,\ldots,p-1$												
[3] $Ibam$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$4a;8h$	$4b;8i$	$4c;8h$	$4d;8i$	$8e;16k$	$8f;16k$	$8g;16k$	$3\times8h$	$3\times8i$	$8j;16k$	$3\times16k$
[p] $Ibam$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$	$4a;$ $\frac{p-1}{2}\times 8h$	$4b;$ $\frac{p-1}{2}\times 8i$	$4c;$ $\frac{p-1}{2}\times 8h$	$4d;$ $\frac{p-1}{2}\times 8i$	$8e;$ $\frac{p-1}{2}\times 16k$	$8f;$ $\frac{p-1}{2}\times 16k$	$8g;$ $\frac{p-1}{2}\times 16k$	$p\times8h$	$p\times8i$	$8j;$ $\frac{p-1}{2}\times 16k$	$p\times16k$
	p = prime > 2; $u = 1,\ldots,p-1$												

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

$Imcb$	$C \to A \to B$	$a \to b \to c \to a$	$\mathbf{a} \to \mathbf{b} \to \mathbf{c} \to \mathbf{a}$	$x \to y \to z \to x$
$Icma$	$A \to C \to B$	$a \leftarrow b \leftarrow c \leftarrow a$	$\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$	$x \leftarrow y \leftarrow z \leftarrow x$

$Ibca$ No. 73 $I\,2_1/b\,2_1/c\,2_1/a$ D_{2h}^{27}

	Axes	Coordinates	8*a*	8*b*	8*c*	8*d*	8*e*	16*f*
I Maximal *translationengleiche* subgroups								
[2] *Iba*2 (45)		$x,y+\frac{1}{4},z$	8*c*	8*c*	8*c*	8*c*	4*a*; 4*b*	2×8*c*
[2] *Ic*2*a* (45)		$x+\frac{1}{4},y,z$	8*c*	8*c*	8*c*	4*a*; 4*b*	8*c*	2×8*c*
≙ *Iba*2	**c**, **a**, **b**	$z,x+\frac{1}{4},y$						
[2] *I*2*cb* (45)		$x,y,z+\frac{1}{4}$	8*c*	8*c*	4*a*; 4*b*	8*c*	8*c*	2×8*c*
≙ *Iba*2	**b**, **c**, **a**	$y,z+\frac{1}{4},x$						
[2] $I2_12_12_1$ (24)			8*d*	8*d*	2×4*a*	2×4*b*	2×4*c*	2×8*d*
[2] *I*2/*c*11 (15)			4*a*; 4*b*	4*c*; 4*d*	2×4*e*	8*f*	8*f*	2×8*f*
≙ *I*12/*a*1	**c**, **a**, **b**	z,x,y						
≙ *C*12/*c*1	−**b**−**c**, **a**, **c**	$-y,x,-y+z$						
[2] *I*12/*a*1 (15)			4*a*; 4*b*	4*c*; 4*d*	8*f*	2×4*e*	8*f*	2×8*f*
≙ *C*12/*c*1	−**a**−**c**, **b**, **a**	$-z,y,x-z$						
[2] *I*112/*b* (15)			4*a*; 4*b*	4*c*; 4*d*	8*f*	8*f*	2×4*e*	2×8*f*
≙ *A*112/*a*	**b**, −**a**−**b**, **c**	$x+y,-x,z$						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] *Pbca* (61)			4*a*; 4*b*	8*c*	8*c*	8*c*	8*c*	2×8*c*
[2] *Pcab* (61)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	8*c*	4*a*; 4*b*	8*c*	8*c*	8*c*	2×8*c*
≙ *Pbca*	**b**, −**a**, **c**	$y+\frac{1}{4},-x-\frac{1}{4},z+\frac{1}{4}$						
≙ *Pbca*	**c**, **b**, −**a**	$z+\frac{1}{4},y+\frac{1}{4},-x-\frac{1}{4}$						
≙ *Pbca*	**a**, **c**, −**b**	$x+\frac{1}{4},z+\frac{1}{4},-y-\frac{1}{4}$						
[2] *Pcca* (54)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	8*f*	4*a*; 4*b*	8*f*	2×4*c*	4*d*; 4*e*	2×8*f*
[2] *Pbaa* (54)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	8*f*	4*a*; 4*b*	4*d*; 4*e*	8*f*	2×4*c*	2×8*f*
≙ *Pcca*	**b**, **c**, **a**	$y+\frac{1}{4},z+\frac{1}{4},x+\frac{1}{4}$						
[2] *Pbcb* (54)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	8*f*	4*a*; 4*b*	2×4*c*	4*d*; 4*e*	8*f*	2×8*f*
≙ *Pcca*	**c**, **a**, **b**	$z+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$						
[2] *Pbab* (54)			4*a*; 4*b*	8*f*	8*f*	4*d*; 4*e*	2×4*c*	2×8*f*
≙ *Pcca*	**a**, −**c**, **b**	$y,-x,z$						
[2] *Pccb* (54)			4*a*; 4*b*	8*f*	2×4*c*	8*f*	4*d*; 4*e*	2×8*f*
≙ *Pcca*	**b**, **a**, −**c**	$y,x,-z$						
[2] *Pcaa* (54)			4*a*; 4*b*	8*f*	4*d*; 4*e*	2×4*c*	8*f*	2×8*f*
≙ *Pcca*	−**c**, **b**, **a**	$-z,y,x$						
Enlarged unit cell, isomorphic								
[3] *Ibca*	3**a**, **b**, **c**	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	8*a*; 16*f*	8*b*; 16*f*	3×8*c*	8*d*; 16*f*	8*e*; 16*f*	3×16*f*
[*p*] *Ibca*	*p***a**, **b**, **c**	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	8*a*; $\frac{p-1}{2}$×16*f*	8*b*; $\frac{p-1}{2}$×16*f*	*p*×8*c*	8*d*; $\frac{p-1}{2}$×16*f*	8*e*; $\frac{p-1}{2}$×16*f*	*p*×16*f*
	p = prime > 2; $u = 1,\ldots,p-1$							
[3] *Ibca*	**a**, 3**b**, **c**	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	8*a*; 16*f*	8*b*; 16*f*	8*c*; 16*f*	3×8*d*	8*e*; 16*f*	3×16*f*
[*p*] *Ibca*	**a**, *p***b**, **c**	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	8*a*; $\frac{p-1}{2}$×16*f*	8*b*; $\frac{p-1}{2}$×16*f*	8*c*; $\frac{p-1}{2}$×16*f*	*p*×8*d*	8*e*; $\frac{p-1}{2}$×16*f*	*p*×16*f*
	p = prime > 2; $u = 1,\ldots,p-1$							
[3] *Ibca*	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	8*a*; 16*f*	8*b*; 16*f*	8*c*; 16*f*	8*d*; 16*f*	3×8*e*	3×16*f*
[*p*] *Ibca*	**a**, **b**, *p***c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	8*a*; $\frac{p-1}{2}$×16*f*	8*b*; $\frac{p-1}{2}$×16*f*	8*c*; $\frac{p-1}{2}$×16*f*	8*d*; $\frac{p-1}{2}$×16*f*	*p*×8*e*	*p*×16*f*
	p = prime > 2; $u = 1,\ldots,p-1$							

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Icab $A \rightarrow B$ $a \rightleftarrows b$ $\mathbf{a} \rightleftarrows -\mathbf{b}$ $x \rightleftarrows -y$

D_{2h}^{28} $\quad I\,2_1/m\,2_1/m\,2_1/a$ $\quad$ No. 74 $\quad$ *Imma*

	Axes	Coordinates	Wyckoff positions									
			$4a$	$4b$	$4c$	$4d$	$4e$	$8f$	$8g$	$8h$	$8i$	$16j$
I Maximal *translationengleiche* subgroups												
[2] $I2mb$ (46)			$4a$	$4a$	$4b$	$4b$	$4b$	$2{\times}4a$	$8c$	$8c$	$2{\times}4b$	$2{\times}8c$
$\widehat{=}$ $Ima2$	$\mathbf{b},\mathbf{c},\mathbf{a}$	y,z,x										
[2] $Im2a$ (46)		$x+\frac{1}{4},y,z+\frac{1}{4}$	$4b$	$4b$	$4a$	$4a$	$4b$	$8c$	$2{\times}4a$	$2{\times}4b$	$8c$	$2{\times}8c$
$\widehat{=}$ $Ima2$	$\mathbf{a},-\mathbf{c},\mathbf{b}$	$x+\frac{1}{4},-z-\frac{1}{4},y$										
[2] $Imm2$ (44)		$x,y+\frac{1}{4},z$	$4d$	$4d$	$4c$	$4c$	$2a;2b$	$8e$	$8e$	$2{\times}4d$	$2{\times}4c$	$2{\times}8e$
[2] $I2_12_12_1$ (24)		$x,y,z+\frac{1}{4}$	$4a$	$4a$	$4b$	$4b$	$4c$	$2{\times}4a$	$2{\times}4b$	$8d$	$8d$	$2{\times}8d$
[2] $I112/b$ (15)			$4a$	$4b$	$4d$	$4c$	$4e$	$8f$	$8f$	$8f$	$8f$	$2{\times}8f$
$\widehat{=}$ $A112/a$	$\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$-x+y,-x,z$										
[2] $I2/m11$ (12)			$2a;2d$	$2b;2c$	$4e$	$4f$	$4i$	$4g;4h$	$8j$	$2{\times}4i$	$8j$	$2{\times}8j$
$\widehat{=}$ $I12/m1$	$\mathbf{c},\mathbf{a},\mathbf{b}$	z,x,y										
$\widehat{=}$ $C12/m1$	$-\mathbf{b}-\mathbf{c},\mathbf{a},\mathbf{c}$	$-y,x,-y+z$										
[2] $I12/m1$ (12)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4e$	$4f$	$2a;2c$	$2b;2d$	$4i$	$8j$	$4g;4h$	$8j$	$2{\times}4i$	$2{\times}8j$
$\widehat{=}$ $C12/m1$	$-\mathbf{a}-\mathbf{c},\mathbf{b},\mathbf{a}$	$-z-\frac{1}{4},y+\frac{1}{4},x-z$										
II Maximal *klassengleiche* subgroups												
Loss of centring translations												
[2] $Pnma$ (62)			$4a$	$4b$	$4c$	$4c$	$4c$	$8d$	$8d$	$8d$	$2{\times}4c$	$2{\times}8d$
[2] $Pmnb$ (62)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4c$	$4c$	$4a$	$4b$	$4c$	$8d$	$8d$	$2{\times}4c$	$8d$	$2{\times}8d$
$\widehat{=}$ $Pnma$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y+\frac{1}{4},-x-\frac{1}{4},z+\frac{1}{4}$										
[2] $Pmna$ (53)			$2a;2d$	$2b;2c$	$4g$	$4g$	$4h$	$4e;4f$	$2{\times}4g$	$2{\times}4h$	$8i$	$2{\times}8i$
[2] $Pnmb$ (53)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4g$	$4g$	$2a;2d$	$2b;2c$	$4h$	$2{\times}4g$	$4e;4f$	$8i$	$2{\times}4h$	$2{\times}8i$
$\widehat{=}$ $Pmna$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y+\frac{1}{4},-x-\frac{1}{4},z+\frac{1}{4}$										
[2] $Pnna$ (52)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4d$	$4d$	$4a$	$4b$	$4c$	$2{\times}4d$	$8e$	$8e$	$8e$	$2{\times}8e$
[2] $Pnnb$ (52)			$4a$	$4b$	$4d$	$4d$	$4c$	$8e$	$2{\times}4d$	$8e$	$8e$	$2{\times}8e$
$\widehat{=}$ $Pnna$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y,-x,z$										
[2] $Pmma$ (51)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4k$	$4k$	$2a;2d$	$2b;2c$	$2e;2f$	$8l$	$4g;4h$	$2{\times}4k$	$4i;4j$	$2{\times}8l$
[2] $Pmmb$ (51)			$2a;2d$	$2b;2c$	$4k$	$4k$	$2e;2f$	$4g;4h$	$8l$	$4i;4j$	$2{\times}4k$	$2{\times}8l$
$\widehat{=}$ $Pmma$	$\mathbf{b},-\mathbf{a},\mathbf{c}$	$y,-x,z$										
Enlarged unit cell, isomorphic												
[3] $Imma$	$3\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,y,z;\ \pm(\frac{1}{3},0,0)$	$4a;8f$	$4b;8f$	$4c;8i$	$4d;8i$	$4e;8i$	$3{\times}8f$	$8g;16j$	$8h;16j$	$3{\times}8i$	$3{\times}16j$
[p] $Imma$	$p\mathbf{a},\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,y,z;\ +(\frac{u}{p},0,0)$	$4a;$	$4b;$	$4c;$	$4d;$	$4e;$	$p{\times}8f$	$8g;$	$8h;$	$p{\times}8i$	$p{\times}16j$
	p = prime > 2; $u=1,\ldots,p-1$		$\frac{p-1}{2}{\times}8f$	$\frac{p-1}{2}{\times}8f$	$\frac{p-1}{2}{\times}8i$	$\frac{p-1}{2}{\times}8i$	$\frac{p-1}{2}{\times}8i$		$\frac{p-1}{2}{\times}16j$	$\frac{p-1}{2}{\times}16j$		
[3] $Imma$	$\mathbf{a},3\mathbf{b},\mathbf{c}$	$x,\frac{1}{3}y,z;\ \pm(0,\frac{1}{3},0)$	$4a;8h$	$4b;8h$	$4d;8g$	$4c;8g$	$4e;8h$	$8f;16j$	$3{\times}8g$	$3{\times}8h$	$8i;16j$	$3{\times}16j$
[p] $Imma$	$\mathbf{a},p\mathbf{b},\mathbf{c}$	$x,\frac{1}{p}y,z;\ +(0,\frac{u}{p},0)$	$4a;$	$4b;$	$4c(d^*);$	$4d(c^*);$	$4e;$	$8f;$	$p{\times}8g$	$p{\times}8h$	$8i;$	$p{\times}16j$
	p = prime > 2; $u=1,\ldots,p-1$		$\frac{p-1}{2}{\times}8h$	$\frac{p-1}{2}{\times}8h$	$\frac{p-1}{2}{\times}8g$	$\frac{p-1}{2}{\times}8g$	$\frac{p-1}{2}{\times}8h$	$\frac{p-1}{2}{\times}16j$			$\frac{p-1}{2}{\times}16j$	
[3] $Imma$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$4a;8h$	$4b;8h$	$4d;8i$	$4c;8i$	$3{\times}4e$	$8f;16j$	$8g;16j$	$3{\times}8h$	$3{\times}8i$	$3{\times}16j$
[p] $Imma$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$4a;$	$4b;$	$4c(d^*);$	$4d(c^*);$	$p{\times}4e$	$8f;$	$8g;$	$p{\times}8h$	$p{\times}8i$	$p{\times}16j$
	p = prime > 2; $u=1,\ldots,p-1$		$\frac{p-1}{2}{\times}8h$	$\frac{p-1}{2}{\times}8h$	$\frac{p-1}{2}{\times}8i$	$\frac{p-1}{2}{\times}8i$		$\frac{p-1}{2}{\times}16j$	$\frac{p-1}{2}{\times}16j$			

* $p=4n-1$

Nonconventional settings

interchange letters and sequences in Hermann–Mauguin symbols, axes and coordinates:

Ibmm	$C\to A\to B$	$a\to b\to c\to a$	$\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$	$x\to y\to z\to x$
Imcm	$A\to C\to B$	$a\leftarrow b\leftarrow c\leftarrow a$	$\mathbf{a}\leftarrow\mathbf{b}\leftarrow\mathbf{c}\leftarrow\mathbf{a}$	$x\leftarrow y\leftarrow z\leftarrow x$

$P4$ No. 75 C_4^1

	Axes	Coordinates	Wyckoff positions 1a	1b	2c	4d
I Maximal *translationengleiche* subgroups						
[2] $P112$ (3)			$1a$	$1d$	$1b; 1c$	$2\times 2e$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $I4$ (79)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2\times 2a$	$4b$	$8c$	$2\times 8c$
[2] $I4$ (79)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4b$	$2\times 2a$	$8c$	$2\times 8c$
[2] $P4_2$ (77)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a$	$2b$	$2\times 2c$	$2\times 4d$
Enlarged unit cell, isomorphic						
[2] $P4$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2\times 1a$	$2\times 1b$	$2\times 2c$	$2\times 4d$
[3] $P4$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times 1a$	$3\times 1b$	$3\times 2c$	$3\times 4d$
[p] $P4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times 1a$	$p\times 1b$	$p\times 2c$	$p\times 4d$
[2] $P4$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$1a; 1b$	$2c$	$4d$	$2\times 4d$
[2] $P4$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$2c$	$1a; 1b$	$4d$	$2\times 4d$
[5] $P4$	$\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x+2y), \frac{1}{5}(-2x+y), z; \pm(\frac{2}{5},\frac{1}{5},0); \pm(\frac{1}{5},\frac{3}{5},0)$	$1a; 4d$	$1b; 4d$	$2c; 2\times 4d$	$5\times 4d$
[5] $P4$	$\mathbf{a}-2\mathbf{b}, 2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x-2y), \frac{1}{5}(2x+y), z; \pm(\frac{3}{5},\frac{1}{5},0); \pm(\frac{1}{5},\frac{2}{5},0)$	$1a; 4d$	$1b; 4d$	$2c; 2\times 4d$	$5\times 4d$
[p] $P4$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b}, \mathbf{c}$ $p = q^2+r^2$ = prime $= 4n+1$; $u = 1,\ldots,p-1$	$\frac{1}{p}(qx-ry), \frac{1}{p}(rx+qy), z;\ +(\frac{uq}{p},\frac{ur}{p},0)$ $q = 2n+1 \geq 1;\ r = \pm 2n' \neq 0;$	$1a; \frac{p-1}{4}\times 4d$	$1b; \frac{p-1}{4}\times 4d$	$2c; \frac{p-1}{2}\times 4d$	$p\times 4d$
[9] $P4$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$1a; 2\times 4d$	$1b; 2\times 4d$	$2c; 4\times 4d$	$9\times 4d$
[p^2] $P4$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime $= 4n-1$; $u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$	$1a; \frac{p^2-1}{4}\times 4d$	$1b; \frac{p^2-1}{4}\times 4d$	$2c; \frac{p^2-1}{2}\times 4d$	$p^2\times 4d$

$P4_1$ No. 76 C_4^2 — C_4^4 No. 78 $P4_3$

	Axes	Coordinates	Wyckoff Positions		Axes	Coordinates
			$4a$			
I Maximal *translationengleiche* subgroups						
[2] $P112_1$ (4)			$2{\times}2a$	[2] $P112_1$ (4)		
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[3] $P4_3$ (78)	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3{\times}4a$	[3] $P4_1$ (76)	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$
[p] $P4_3$ (78)	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime = $4n-1$; $u=1,\ldots,p-1$	$p{\times}4a$	[p] $P4_1$ (76)	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime = $4n-1$; $u=1,\ldots,p-1$
[5] $P4_1$	**a**, **b**, 5**c**	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});\ \pm(0,0,\frac{2}{5})$	$5{\times}4a$	[5] $P4_3$	**a**, **b**, 5**c**	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});\ \pm(0,0,\frac{2}{5})$
[p] $P4_1$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime = $4n+1$; $u=1,\ldots,p-1$	$p{\times}4a$	[p] $P4_3$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime = $4n+1$; $u=1,\ldots,p-1$
[2] $P4_1$	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;\ +(\frac{1}{2},\frac{1}{2},0)$	$2{\times}4a$	[2] $P4_3$	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;\ +(\frac{1}{2},\frac{1}{2},0)$
[2] $P4_1$	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;\ +(\frac{1}{2},\frac{1}{2},0)$	$2{\times}4a$	[2] $P4_3$	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;\ +(\frac{1}{2},\frac{1}{2},0)$
[5] $P4_1$	**a**+2**b**, −2**a**+**b**, **c**	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z;$ $\pm(\frac{1}{5},\frac{3}{5},0);\ \pm(\frac{2}{5},\frac{1}{5},0)$	$5{\times}4a$	[5] $P4_3$	**a**+2**b**, −2**a**+**b**, **c**	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z;$ $\pm(\frac{1}{5},\frac{3}{5},0);\ \pm(\frac{2}{5},\frac{1}{5},0)$
[5] $P4_1$	**a**−2**b**, 2**a**+**b**, **c**	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z;$ $\pm(\frac{1}{5},\frac{2}{5},0);\ \pm(\frac{3}{5},\frac{1}{5},0)$	$5{\times}4a$	[5] $P4_3$	**a**−2**b**, 2**a**+**b**, **c**	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z;$ $\pm(\frac{1}{5},\frac{2}{5},0);\ \pm(\frac{3}{5},\frac{1}{5},0)$
[p] $P4_1$	q**a**−r**b**, r**a**+q**b**, **c**	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z;+(\frac{uq}{p},\frac{ur}{p},0)$ $q=2n+1\geq 1$; $r=\pm 2n'\neq 0$ $p=q^2+r^2$ = prime = $4n+1$; $u=1,\ldots,p-1$	$p{\times}4a$	[p] $P4_3$	q**a**−r**b**, r**a**+q**b**, **c**	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z;+(\frac{uq}{p},\frac{ur}{p},0)$ $q=2n+1\geq 1$; $r=\pm 2n'\neq 0$ $p=q^2+r^2$ = prime = $4n+1$; $u=1,\ldots,p-1$
[9] $P4_1$	3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z;\ \pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$	$9{\times}4a$	[9] $P4_3$	3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z;\ \pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$
[p^2] $P4_1$	p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$ p = prime = $4n-1$; $u,v=1,\ldots,p-1$	$p^2{\times}4a$	[p^2] $P4_3$	p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$ p = prime = $4n-1$; $u,v=1,\ldots,p-1$

$P4_2$ No. 77 C_4^3

Axes	Coordinates		Wyckoff positions			
			$2a$	$2b$	$2c$	$4d$
I Maximal *translationengleiche* subgroups						
[2] $P112$ (3)			$2\times1a$	$2\times1d$	$1b; 1c$	$2\times2e$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $I4_1$ (80)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}, \frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$8b$	$8b$	$2\times4a$	$2\times8b$
[2] $I4_1$ (80)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y)-\frac{1}{4}, \frac{1}{2}(x+y)+\frac{1}{4}, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$8b$	$8b$	$2\times4a$	$2\times8b$
[2] $P4_3$ (78)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4a$	$4a$	$2\times4a$
[2] $P4_1$ (76)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4a$	$4a$	$2\times4a$
Enlarged unit cell, isomorphic						
[3] $P4_2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times2c$	$3\times4d$
[p] $P4_2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime > 2; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times2a$	$p\times2b$	$p\times2c$	$p\times4d$
[2] $P4_2$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$2a; 2b$	$2\times2c$	$4d$	$2\times4d$
[2] $P4_2$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$2\times2c$	$2a; 2b$	$4d$	$2\times4d$
[5] $P4_2$	$\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x+2y), \frac{1}{5}(-2x+y), z;\ \pm(\frac{2}{5},\frac{1}{5},0);\ \pm(\frac{1}{5},\frac{3}{5},0)$	$2a; 2\times4d$	$2b; 2\times4d$	$2c; 2\times4d$	$5\times4d$
[5] $P4_2$	$\mathbf{a}-2\mathbf{b}, 2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x-2y), \frac{1}{5}(2x+y), z;\ \pm(\frac{3}{5},\frac{1}{5},0);\ \pm(\frac{1}{5},\frac{2}{5},0)$	$2a; 2\times4d$	$2b; 2\times4d$	$2c; 2\times4d$	$5\times4d$
[p] $P4_2$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b}, \mathbf{c}$ $p = q^2+r^2$ = prime $= 4n+1$; $u = 1,\ldots,p-1$	$\frac{1}{p}(qx-ry), \frac{1}{p}(rx+qy), z;\ +(\frac{uq}{p},\frac{ur}{p},0)$ $q = 2n+1 \geq 1$; $r = \pm 2n' \neq 0$;	$2a; \frac{p-1}{2}\times4d$	$2b; \frac{p-1}{2}\times4d$	$2c; \frac{p-1}{2}\times4d$	$p\times4d$
[9] $P4_2$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z;\ \pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$	$2a; 4\times4d$	$2b; 4\times4d$	$2c; 4\times4d$	$9\times4d$
[p^2] $P4_2$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime $= 4n-1$; $u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$	$2a; \frac{p^2-1}{2}\times4d$	$2b; \frac{p^2-1}{2}\times4d$	$2c; \frac{p^2-1}{2}\times4d$	$p^2\times4d$

C_4^5 No. 79 $I4$

	Axes	Coordinates	Wyckoff positions		
			$2a$	$4b$	$8c$
I Maximal *translationengleiche* subgroups					
[2] $I112$ (5)			$2a$	$2\times2b$	$2\times4c$
$\widehat{=} A112$	**a**, −**a**+**b**, **c**	$x+y, y, z$			
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $P4_2$ (77)		$x+\frac{1}{2}, y, z$	$2c$	$2a; 2b$	$2\times4d$
[2] $P4$ (75)			$1a; 1b$	$2\times2c$	$2\times4d$
Enlarged unit cell, isomorphic					
[3] $I4$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times4b$	$3\times8c$
[p] $I4$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times2a$	$p\times4b$	$p\times8c$
	p = prime > 2; $u = 1,\ldots,p-1$				
[5] $I4$	**a**+2**b**, −2**a**+**b**, **c**	$\frac{1}{5}(x+2y), \frac{1}{5}(-2x+y), z$; $\pm(\frac{2}{5},\frac{1}{5},0)$; $\pm(\frac{1}{5},\frac{3}{5},0)$	$2a; 8c$	$4b; 2\times8c$	$5\times8c$
[5] $I4$	**a**−2**b**, 2**a**+**b**, **c**	$\frac{1}{5}(x-2y), \frac{1}{5}(2x+y), z$; $\pm(\frac{3}{5},\frac{1}{5},0)$; $\pm(\frac{1}{5},\frac{2}{5},0)$	$2a; 8c$	$4b; 2\times8c$	$5\times8c$
[p] $I4$	q**a**−r**b**, r**a**+q**b**, **c**	$\frac{1}{p}(qx-ry), \frac{1}{p}(rx+qy), z$; $+(\frac{uq}{p},\frac{ur}{p},0)$; $q = 2n+1 \geq 1$; $r = \pm2n' \neq 0$;	$2a; \frac{p-1}{4}\times8c$	$4b; \frac{p-1}{2}\times8c$	$p\times4d$
	$p = q^2+r^2$ = prime $= 4n+1$; $u = 1,\ldots,p-1$				
[9] $I4$	3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a; 2\times8c$	$4b; 4\times8c$	$9\times8c$
[p^2] $I4$	p**a**, p**b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a; \frac{p^2-1}{4}\times8c$	$4b; \frac{p^2-1}{2}\times8c$	$p^2\times4d$
	p = prime $= 4n-1$; $u, v = 1,\ldots,p-1$				

$I4_1$ No. 80 C_4^6

	Axes	Coordinates	Wyckoff positions	
			$4a$	$8b$
I Maximal *translationengleiche* subgroups				
[2] $I112$ (5)			$2a; 2b$	$2\times 4c$
$\widehat{=} A112$	$\mathbf{a}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$x+y, y, z$		
II Maximal *klassengleiche* subgroups				
Loss of centring translations				
[2] $P4_3$ (78)		$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4a$	$2\times 4a$
[2] $P4_1$ (76)		$x+\frac{1}{4}, y-\frac{1}{4}, z$	$4a$	$2\times 4a$
Enlarged unit cell, isomorphic				
[3] $I4_1$	$\mathbf{b}, -\mathbf{a}, 3\mathbf{c}$	$y, -x, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times 4a$	$3\times 8b$
[p] $I4_1$	$\mathbf{b}, -\mathbf{a}, p\mathbf{c}$	$y, -x, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times 4a$	$p\times 8b$
	$p = \text{prime} = 4n-1$; $u = 1,\ldots,p-1$			
[5] $I4_1$	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z$; $\pm(0,0,\frac{1}{5})$; $\pm(0,0,\frac{2}{5})$	$5\times 4a$	$5\times 8b$
[p] $I4_1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times 4a$	$p\times 8b$
	$p = \text{prime} = 4n+1$; $u = 1,\ldots,p-1$			
[5] $I4_1$	$\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x+2y), \frac{1}{5}(-2x+y), z$; $\pm(\frac{1}{5},\frac{3}{5},0)$; $\pm(\frac{2}{5},\frac{1}{5},0)$	$4a; 2\times 8b$	$5\times 8b$
[5] $I4_1$	$\mathbf{a}-2\mathbf{b}, 2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x-2y), \frac{1}{5}(2x+y), z$; $\pm(\frac{1}{5},\frac{2}{5},0)$; $\pm(\frac{3}{5},\frac{1}{5},0)$	$4a; 2\times 8b$	$5\times 8b$
[p] $I4_1$	$q\mathbf{a}-r\mathbf{b}$,	$\frac{1}{p}(qx-ry), \frac{1}{p}(rx+qy), z$; $+(\frac{uq}{p},\frac{ur}{p},0)$	$4a; \frac{p-1}{2}\times 8b$	$p\times 8b$
	$r\mathbf{a}+q\mathbf{b}, \mathbf{c}$	$q = 2n+1 \geq 1$; $r = \pm 2n' \neq 0$;		
	$p = q^2+r^2 = \text{prime} = 4n+1$; $u = 1,\ldots,p-1$			
[9] $I4_1$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$4a; 4\times 8b$	$9\times 8b$
[p^2] $I4_1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$4a; \frac{p^2-1}{2}\times 8b$	$p^2\times 8b$
	$p = \text{prime} = 4n-1$; $u, v = 1,\ldots,p-1$			

S_4^1 No. 81 $P\bar{4}$

Subgroup	Axes	Coordinates	$1a$	$1b$	$1c$	$1d$	$2e$	$2f$	$2g$	$4h$
I Maximal *translationengleiche* subgroups										
[2] $P112\,(3)$			$1a$	$1a$	$1d$	$1d$	$2{\times}1a$	$2{\times}1d$	$1b;1c$	$2{\times}2e$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $I\bar{4}$ (82)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a;2b$	$4e$	$4f$	$2c;2d$	$2{\times}4e$	$2{\times}4f$	$8g$	$2{\times}8g$
[2] $I\bar{4}$ (82)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4e$	$2a;2b$	$2c;2d$	$4f$	$2{\times}4e$	$2{\times}4f$	$8g$	$2{\times}8g$
Enlarged unit cell, isomorphic										
[2] $P\bar{4}$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a;1b$	$2e$	$1c;1d$	$2f$	$2{\times}2e$	$2{\times}2f$	$2{\times}2g$	$2{\times}4h$
[2] $P\bar{4}$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2e$	$1a;1b$	$2f$	$1c;1d$	$2{\times}2e$	$2{\times}2f$	$2{\times}2g$	$2{\times}4h$
[3] $P\bar{4}$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a;2e$	$1b;2e$	$1c;2f$	$1d;2f$	$3{\times}2e$	$3{\times}2f$	$3{\times}2g$	$3{\times}4h$
[p] $P\bar{4}$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$; $p=$ prime >2; $u=1,\ldots,p-1$	$1a;\frac{p-1}{2}{\times}2e$	$1b;\frac{p-1}{2}{\times}2e$	$1c;\frac{p-1}{2}{\times}2f$	$1d;\frac{p-1}{2}{\times}2f$	$p{\times}2e$	$p{\times}2f$	$p{\times}2g$	$p{\times}4h$
[2] $P\bar{4}$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a;1c$	$1b;1d$	$2g$	$2g$	$2e;2f$	$2{\times}2g$	$4h$	$2{\times}4h$
[2] $P\bar{4}$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2g$	$2g$	$1a;1c$	$1b;1d$	$2{\times}2g$	$2e;2f$	$4h$	$2{\times}4h$
[5] $P\bar{4}$	$\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z$; $\pm(\frac{1}{5},\frac{3}{5},0)$; $\pm(\frac{2}{5},\frac{1}{5},0)$	$1a;4h$	$1b;4h$	$1c;4h$	$1d;4h$	$2e;2{\times}4h$	$2f;2{\times}4h$	$2g;2{\times}4h$	$5{\times}4h$
[5] $P\bar{4}$	$\mathbf{a}-2\mathbf{b}$, $2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z$; $\pm(\frac{1}{5},\frac{2}{5},0)$; $\pm(\frac{3}{5},\frac{1}{5},0)$	$1a;4h$	$1b;4h$	$1c;4h$	$1d;4h$	$2e;2{\times}4h$	$2f;2{\times}4h$	$2g;2{\times}4h$	$5{\times}4h$
[p] $P\bar{4}$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z$; $+(\frac{uq}{p},\frac{ur}{p},0)$; $p=q^2+r^2=$ prime $=4n+1$; $q=2n+1\geq 1$; $r=\pm 2n'\neq 0$; $u=1,\ldots,p-1$	$1a;\frac{p-1}{4}{\times}4h$	$1b;\frac{p-1}{4}{\times}4h$	$1c;\frac{p-1}{4}{\times}4h$	$1d;\frac{p-1}{4}{\times}4h$	$2e;\frac{p-1}{2}{\times}4h$	$2f;\frac{p-1}{2}{\times}4h$	$2g;\frac{p-1}{2}{\times}4h$	$p{\times}4h$
[9] $P\bar{4}$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;2{\times}4h$	$1b;2{\times}4h$	$1c;2{\times}4h$	$1d;2{\times}4h$	$2e;4{\times}4h$	$2f;4{\times}4h$	$2g;4{\times}4h$	$9{\times}4h$
[p^2] $P\bar{4}$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$; $p=$ prime $=4n-1$; $u,v=1,\ldots,p-1$	$1a;\frac{p^2-1}{4}{\times}4h$	$1b;\frac{p^2-1}{4}{\times}4h$	$1c;\frac{p^2-1}{4}{\times}4h$	$1d;\frac{p^2-1}{4}{\times}4h$	$2e;\frac{p^2-1}{2}{\times}4h$	$2f;\frac{p^2-1}{2}{\times}4h$	$2g;\frac{p^2-1}{2}{\times}4h$	$p^2{\times}4h$

$I\bar{4}$ No. 82 S_4^2

Axes	Coordinates		Wyckoff positions						
			$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$8g$
I Maximal *translationengleiche* subgroups									
[2] $I112$ (5)			$2a$	$2a$	$2b$	$2b$	$2\times 2a$	$2\times 2b$	$2\times 4c$
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $P\bar{4}$ (81)			$1a;1d$	$1b;1c$	$2g$	$2g$	$2e;2f$	$2\times 2g$	$2\times 4h$
[2] $P\bar{4}$ (81)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2g$	$2g$	$1a;1d$	$1b;1c$	$2\times 2g$	$2e;2f$	$2\times 4h$
Enlarged unit cell, isomorphic									
[3] $I\bar{4}$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ +(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$2d;4f$	$2c;4f$	$3\times 4e$	$3\times 4f$	$3\times 8g$
[p] $I\bar{4}$	**a**, **b**, p**c** p = prime > 2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times 4e$	$2b$; $\frac{p-1}{2}\times 4e$	$2c(d^*)$; $\frac{p-1}{2}\times 4f$	$2d(c^*)$; $\frac{p-1}{2}\times 4f$	$p\times 4e$	$p\times 4f$	$p\times 8g$
[5] $I\bar{4}$	**a**+2**b**, −2**a**+**b**, **c**	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z;$ $\pm(\frac{1}{5},\frac{3}{5},0);\pm(\frac{2}{5},\frac{1}{5},0)$	$2a;8g$	$2b;8g$	$2c;8g$	$2d;8g$	$4e;2\times 8g$	$4f;2\times 8g$	$5\times 8g$
[5] $I\bar{4}$	**a**−2**b**, 2**a**+**b**, **c**	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z;$ $\pm(\frac{1}{5},\frac{2}{5},0);\pm(\frac{3}{5},\frac{1}{5},0)$	$2a;8g$	$2b;8g$	$2c;8g$	$2d;8g$	$4e;2\times 8g$	$4f;2\times 8g$	$5\times 8g$
[p] $I\bar{4}$	q**a**−r**b**, r**a**+q**b**, **c** $p=q^2+r^2$ = prime $=4n+1$; $q=2n+1\geq 1$; $r=\pm 2n'\neq 0$;	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z;$ $+(\frac{uq}{p},\frac{ur}{p},0)$ $u=1,\ldots,p-1$	$2a$; $\frac{p-1}{4}\times 8g$	$2b$; $\frac{p-1}{4}\times 8g$	$2c$; $\frac{p-1}{4}\times 8g$	$2d$; $\frac{p-1}{4}\times 8g$	$4e$; $\frac{p-1}{2}\times 8g$	$4f$; $\frac{p-1}{2}\times 8g$	$p\times 8g$
[9] $I\bar{4}$	3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times 8g$	$2b;2\times 8g$	$2c;2\times 8g$	$2d;2\times 8g$	$4e;4\times 8g$	$4f;4\times 8g$	$9\times 8g$
[p^2] $I\bar{4}$	p**a**, p**b**, **c** p = prime $=4n-1$; $u,v=1,\ldots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$2a$; $\frac{p^2-1}{4}\times 8g$	$2b$; $\frac{p^2-1}{4}\times 8g$	$2c$; $\frac{p^2-1}{4}\times 8g$	$2d$; $\frac{p^2-1}{4}\times 8g$	$4e$; $\frac{p^2-1}{2}\times 8g$	$4f$; $\frac{p^2-1}{2}\times 8g$	$p^2\times 8g$

$^*p=4n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 83, pp. 557–558.

C_{4h}^1 No. 83 $P4/m$

	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$1c$	$1d$	$2e$	$2f$	$2g$	$2h$	$4i$	$4j$	$4k$ $8l$
I Maximal *translationengleiche* subgroups													
[2] $P\bar{4}$ (81)			$1a$	$1b$	$1c$	$1d$	$2g$	$2g$	$2e$	$2f$	$2{\times}2g$	$4h$	$4h$ $2{\times}4h$
[2] $P4$ (75)			$1a$	$1a$	$1b$	$1b$	$2c$	$2c$	$2{\times}1a$	$2{\times}1b$	$2{\times}2c$	$4d$	$4d$ $2{\times}4d$
[2] $P112/m$ (10)			$1a$	$1b$	$1g$	$1h$	$1c; 1d$	$1e; 1f$	$2i$	$2l$	$2j; 2k$	$2{\times}2m$	$2{\times}2n$ $2{\times}4o$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**													
[2] $I4/m$ (87)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$2a; 2b$	$4e$	$4c$	$4d$	$8h$	$8f$	$2{\times}4e$	$8g$	$16i$	$2{\times}8h$	$16i$ $2{\times}16i$
[2] $I4/m$ (87)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$4c$	$4d$	$2a; 2b$	$4e$	$8h$	$8f$	$8g$	$2{\times}4e$	$16i$	$2{\times}8h$	$16i$ $2{\times}16i$
[2] $I4/m$ (87)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	$4e$	$2a; 2b$	$4d$	$4c$	$8f$	$8h$	$2{\times}4e$	$8g$	$16i$	$16i$	$2{\times}8h$ $2{\times}16i$
[2] $I4/m$ (87)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y),$ $\frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4d$	$4c$	$4e$	$2a; 2b$	$8f$	$8h$	$8g$	$2{\times}4e$	$16i$	$16i$	$2{\times}8h$ $2{\times}16i$
[2] $P4/n$ (85)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	origin 1: $\frac{1}{2}(x-y),$ $\frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4},$ $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	$2a$	$2b$	$2c$	$2c$	$4d$	$4e$	$4f$	$2{\times}2c$	$8g$	$8g$	$8g$ $2{\times}8g$
[2] $P4/n$ (85)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2},$ $\frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4},$ $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	$2c$	$2c$	$2a$	$2b$	$4d$	$4e$	$2{\times}2c$	$4f$	$8g$	$8g$	$8g$ $2{\times}8g$
[2] $P4_2/m$ (84)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2e$	$2b$	$2f$	$2c; 2d$	$4i$	$4g$	$4h$	$2{\times}4i$	$2{\times}4j$	$8k$ $2{\times}8k$
[2] $P4_2/m$ (84)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$2e$	$2a$	$2f$	$2b$	$4i$	$2c; 2d$	$4g$	$4h$	$2{\times}4i$	$8k$	$2{\times}4j$ $2{\times}8k$

	Axes	Coordinates	$1a$	$1b$	$1c$	$1d$	$2e$ $4i$	$2f$ $4j$	$2g$ $4k$	$2h$ $8l$
Enlarged unit cell, isomorphic										
[2] $P4/m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$1a; 1b$	$2g$	$1c; 1d$	$2h$	$2e; 2f$ $2\times4i$	$4i$ $4j; 4k$	$2\times2g$ $8l$	$2\times2h$ $2\times8l$
[2] $P4/m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$2g$	$1a; 1b$	$2h$	$1c; 1d$	$4i$ $2\times4i$	$2e; 2f$ $8l$	$2\times2g$ $4j; 4k$	$2\times2h$ $2\times8l$
[3] $P4/m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$1a; 2g$	$1b; 2g$	$1c; 2h$	$1d; 2h$	$2e; 4i$ $3\times4i$	$2f; 4i$ $4j; 8l$	$3\times2g$ $4k; 8l$	$3\times2h$ $3\times8l$
[p] $P4/m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime > 2; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$1a$; $\frac{p-1}{2}\times2g$	$1b$; $\frac{p-1}{2}\times2g$	$1c$; $\frac{p-1}{2}\times2h$	$1d$; $\frac{p-1}{2}\times2h$	$2e$; $\frac{p-1}{2}\times4i$ $p\times4i$	$2f$; $\frac{p-1}{2}\times4i$ $4j$; $\frac{p-1}{2}\times8l$	$p\times2g$ $4k$; $\frac{p-1}{2}\times8l$	$p\times2h$ $p\times8l$
[2] $P4/m$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a; 1c$	$1b; 1d$	$2e$	$2f$	$4j$ $8l$	$4k$ $2\times4j$	$2g; 2h$ $2\times4k$	$4i$ $2\times8l$
[2] $P4/m$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2e$	$2f$	$1a; 1c$	$1b; 1d$	$4j$ $8l$	$4k$ $2\times4j$	$4i$ $2\times4k$	$2g; 2h$ $2\times8l$
[5] $P4/m$	$\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x+2y), \frac{1}{5}(-2x+y), z$; $\pm(\frac{1}{5},\frac{3}{5},0); \pm(\frac{2}{5},\frac{1}{5},0)$	$1a; 4j$	$1b; 4k$	$1c; 4j$	$1d; 4k$	$2e; 2\times4j$ $4i; 2\times8l$	$2f; 2\times4k$ $5\times4j$	$2g; 8l$ $5\times4k$	$2h; 8l$ $5\times8l$
[5] $P4/m$	$\mathbf{a}-2\mathbf{b}, 2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{5}(x-2y), \frac{1}{5}(2x+y), z$; $\pm(\frac{1}{5},\frac{2}{5},0); \pm(\frac{3}{5},\frac{1}{5},0)$	$1a; 4j$	$1b; 4k$	$1c; 4j$	$1d; 4k$	$2e; 2\times4j$ $4i; 2\times8l$	$2f; 2\times4k$ $5\times4j$	$2g; 8l$ $5\times4k$	$2h; 8l$ $5\times8l$
[p] $P4/m$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b}, \mathbf{c}$ $p = q^2+r^2$ = prime = $4n+1$; $q = 2n+1 \geq 1$; $r = \pm2n' \neq 0$;	$\frac{1}{p}(qx-ry), \frac{1}{p}(rx+qy), z$; $+(\frac{uq}{p},\frac{ur}{p},0)$ $u = 1, \ldots, p-1$	$1a$; $\frac{p-1}{4}\times4j$	$1b$; $\frac{p-1}{4}\times4k$	$1c$; $\frac{p-1}{4}\times4j$	$1d$; $\frac{p-1}{4}\times4k$	$2e$; $\frac{p-1}{2}\times4j$ $4i$; $\frac{p-1}{2}\times8l$	$2f$; $\frac{p-1}{2}\times4k$ $p\times4j$	$2g$; $\frac{p-1}{4}\times8l$ $p\times4k$	$2h$; $\frac{p-1}{4}\times8l$ $p\times8l$
[9] $P4/m$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$1a; 2\times4j$	$1b; 2\times4k$	$1c; 2\times4j$	$1d; 2\times4k$	$2e; 4\times4j$ $4i; 4\times8l$	$2f; 4\times4k$ $9\times4j$	$2g; 2\times8l$ $9\times4k$	$2h; 2\times8l$ $9\times8l$
[p^2] $P4/m$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime = $4n-1$;	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$ $u, v = 1, \ldots, p-1$	$1a$; $\frac{p^2-1}{4}\times4j$	$1b$; $\frac{p^2-1}{4}\times4k$	$1c$; $\frac{p^2-1}{4}\times4j$	$1d$; $\frac{p^2-1}{4}\times4k$	$2e$; $\frac{p^2-1}{2}\times4j$ $4i$; $\frac{p^2-1}{2}\times8l$	$2f$; $\frac{p^2-1}{2}\times4k$ $p^2\times4j$	$2g$; $\frac{p^2-1}{4}\times8l$ $p^2\times4k$	$2h$; $\frac{p^2-1}{4}\times8l$ $p^2\times8l$

C_{4h}^{2} No. 84 $P4_2/m$

	Axes	Coordinates	Wyckoff positions							
			$2a$	$2b$	$2c$	$2d$	$2e$	$2f$ $4i$	$4g$ $4j$	$4h$ $8k$
I Maximal *translationengleiche* subgroups										
[2] $P\bar{4}$ (81)		$x,y,z+\frac{1}{4}$	$2e$	$2f$	$2g$	$2g$	$1a;1b$	$1c;1d$ $2{\times}2g$	$2{\times}2e$ $4h$	$2{\times}2f$ $2{\times}4h$
[2] $P4_2$ (77)			$2a$	$2b$	$2c$	$2c$	$2a$	$2b$ $2{\times}2c$	$2{\times}2a$ $4d$	$2{\times}2b$ $2{\times}4d$
[2] $P112/m$ (10)			$1a;1b$	$1g;1h$	$1d;1f$	$1c;1e$	$2i$	$2l$ $2j;2k$	$2{\times}2i$ $2m;2n$	$2{\times}2l$ $2{\times}4o$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $P4_2/n$ (86)	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	origin 1: $\frac{1}{2}(x-y),\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4},\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	$4f$	$4e$	$4d$	$4c$	$2a;2b$	$4e$ $8g$	$2{\times}4f$ $8g$	$2{\times}4e$ $2{\times}8g$
[2] $P4_2/n$ (86)	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4},\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	$4e$	$4f$	$4c$	$4d$	$4e$	$2a;2b$ $8g$	$2{\times}4e$ $8g$	$2{\times}4f$ $2{\times}8g$
Enlarged unit cell, isomorphic										
[3] $P4_2/m$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4g$	$2b;4h$	$2c;4i$	$2d;4i$	$2e;4g$	$2f;4h$ $3{\times}4i$	$3{\times}4g$ $4j;8k$	$3{\times}4h$ $3{\times}8k$
[p] $P4_2/m$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}{\times}4g$	$2b;$ $\frac{p-1}{2}{\times}4h$	$2c;$ $\frac{p-1}{2}{\times}4i$	$2d;$ $\frac{p-1}{2}{\times}4i$	$2e;$ $\frac{p-1}{2}{\times}4g$	$2f;$ $\frac{p-1}{2}{\times}4h$ $p{\times}4i$	$p{\times}4g$ $4j;$ $\frac{p-1}{2}{\times}8k$	$p{\times}4h$ $p{\times}8k$
[2] $P4_2/m$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2b$	$2c;2d$	$4j$	$4j$	$2e;2f$	$4i$ $8k$	$4g;4h$ $2{\times}4j$	$2{\times}4i$ $2{\times}8k$
[2] $P4_2/m$	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2c;2d$	$2a;2b$	$4j$	$4j$	$4i$	$2e;2f$ $8k$	$2{\times}4i$ $2{\times}4j$	$4g;4h$ $2{\times}8k$
[5] $P4_2/m$	$\mathbf{a}+2\mathbf{b},$ $-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z;$ $\pm(\frac{1}{5},\frac{3}{5},0);\pm(\frac{2}{5},\frac{1}{5},0)$	$2a;2{\times}4j$	$2b;2{\times}4j$	$2c;2{\times}4j$	$2d;2{\times}4j$	$2e;8k$	$2f;8k$ $4i;2{\times}8k$	$4g;2{\times}8k$ $5{\times}4j$	$4h;2{\times}8k$ $5{\times}8k$
[5] $P4_2/m$	$\mathbf{a}-2\mathbf{b},$ $2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z;$ $\pm(\frac{1}{5},\frac{2}{5},0);\pm(\frac{3}{5},\frac{1}{5},0)$	$2a;2{\times}4j$	$2b;2{\times}4j$	$2c;2{\times}4j$	$2d;2{\times}4j$	$2e;8k$	$2f;8k$ $4i;2{\times}8k$	$4g;2{\times}8k$ $5{\times}4j$	$4h;2{\times}8k$ $5{\times}8k$
[p] $P4_2/m$	$q\mathbf{a}-r\mathbf{b},$ $r\mathbf{a}+q\mathbf{b},\mathbf{c}$	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z;$ $+(\frac{uq}{p},\frac{ur}{p},0)$ $p=q^2+r^2=$ prime $=4n+1$; $q=2n+1\geq 1$; $r=\pm 2n'\neq 0$; $u=1,\ldots,p-1$	$2a;$ $\frac{p-1}{2}{\times}4j$	$2b;$ $\frac{p-1}{2}{\times}4j$	$2c;$ $\frac{p-1}{2}{\times}4j$	$2d;$ $\frac{p-1}{2}{\times}4j$	$2e;$ $\frac{p-1}{4}{\times}8k$	$2f;$ $\frac{p-1}{4}{\times}8k$ $4i;$ $\frac{p-1}{2}{\times}8k$	$4g;$ $\frac{p-1}{2}{\times}8k$ $p{\times}4j$	$4h;$ $\frac{p-1}{2}{\times}8k$ $p{\times}8k$
[9] $P4_2/m$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;\pm(\frac{1}{3},0,0);$ $\pm(0,\frac{1}{3},0);\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4{\times}4j$	$2b;4{\times}4j$	$2c;4{\times}4j$	$2d;4{\times}4j$	$2e;2{\times}8k$	$2f;2{\times}8k$ $4i;4{\times}8k$	$4g;4{\times}8k$ $9{\times}4j$	$4h;4{\times}8k$ $9{\times}8k$
[p^2] $P4_2/m$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $p=$ prime $=4n-1$; $u,v=1,\ldots,p-1$	$2a;$ $\frac{p^2-1}{2}{\times}4j$	$2b;$ $\frac{p^2-1}{2}{\times}4j$	$2c;$ $\frac{p^2-1}{2}{\times}4j$	$2d;$ $\frac{p^2-1}{2}{\times}4j$	$2e;$ $\frac{p^2-1}{4}{\times}8k$	$2f;$ $\frac{p^2-1}{4}{\times}8k$ $4i;$ $\frac{p^2-1}{2}{\times}8k$	$4g;$ $\frac{p^2-1}{2}{\times}8k$ $p^2{\times}4j$	$4h;$ $\frac{p^2-1}{2}{\times}8k$ $p^2{\times}8k$

$P4/n$ No. 85 C_{4h}^{3}

Subgroup	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$2c$	$4d$	$4e$	$4f$	$8g$
I Maximal *translationengleiche* subgroups										
[2] $P\bar{4}$ (81)			$x+\frac{1}{4}, y-\frac{1}{4}, z$	$1a; 1c$	$1b; 1d$	$2g$	$4h$	$4h$	$2e; 2f$	$2\times4h$
[2] $P4$ (75)		$x+\frac{1}{2}, y, z$	$x+\frac{1}{4}, y+\frac{1}{4}, z$	$2c$	$2c$	$1a; 1b$	$4d$	$4d$	$2\times2c$	$2\times4d$
[2] $P112/n$ (13)		$x+\frac{1}{4}, y-\frac{1}{4}, z$		$2f$	$2f$	$2e$	$2a; 2d$	$2b; 2c$	$2\times2f$	$2\times4g$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $P4_2/n$ (86)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$x+\frac{1}{2}, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2a; 2b$	$4f$	$4e$	$8g$	$4c; 4d$	$2\times4f$	$2\times8g$
[2] $P4_2/n$ (86)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$x+\frac{1}{2}, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4f$	$2a; 2b$	$4e$	$4c; 4d$	$8g$	$2\times4f$	$2\times8g$
Enlarged unit cell, isomorphic										
[2] $P4/n$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$		$2a; 2b$	$4f$	$2\times2c$	$4d; 4e$	$8g$	$2\times4f$	$2\times8g$
[2] $P4/n$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$		$4f$	$2a; 2b$	$2\times2c$	$8g$	$4d; 4e$	$2\times4f$	$2\times8g$
[3] $P4/n$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$		$2a; 4f$	$2b; 4f$	$3\times2c$	$4d; 8g$	$4e; 8g$	$3\times4f$	$3\times8g$
[p] $P4/n$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$; p = prime > 2; $u = 1, \dots, p-1$		$2a$; $\frac{p-1}{2}\times4f$	$2b$; $\frac{p-1}{2}\times4f$	$p\times2c$	$4d$; $\frac{p-1}{2}\times8g$	$4e$; $\frac{p-1}{2}\times8g$	$p\times4f$	$p\times8g$
[5] $P4/n$	$\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x+2y), \frac{1}{5}(-2x+y), z$; $\pm(\frac{1}{5},\frac{3}{5},0)$; $\pm(\frac{2}{5},\frac{1}{5},0)$		$2a; 8g$	$2b; 8g$	$2c; 8g$	$4d; 2\times8g$	$4e; 2\times8g$	$4f; 2\times8g$	$5\times8g$
[5] $P4/n$	$\mathbf{a}-2\mathbf{b}$, $2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x-2y), \frac{1}{5}(2x+y), z$; $\pm(\frac{1}{5},\frac{2}{5},0)$; $\pm(\frac{3}{5},\frac{1}{5},0)$		$2a; 8g$	$2b; 8g$	$2c; 8g$	$4d; 2\times8g$	$4e; 2\times8g$	$4f; 2\times8g$	$5\times8g$
[p] $P4/n$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}(qx-ry), \frac{1}{p}(rx+qy), z$; $+(\frac{uq}{p},\frac{ur}{p},0)$; $p = q^2+r^2$ = prime $= 4n+1$; $q = 2n+1 \geq 1$; $r = \pm2n' \neq 0$; $u = 1, \dots, p-1$		$2a$; $\frac{p-1}{4}\times8g$	$2b$; $\frac{p-1}{4}\times8g$	$2c$; $\frac{p-1}{4}\times8g$	$4d$; $\frac{p-1}{2}\times8g$	$4e$; $\frac{p-1}{2}\times8g$	$4f$; $\frac{p-1}{2}\times8g$	$p\times8g$
[9] $P4/n$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$		$2a; 2\times8g$	$2b; 2\times8g$	$2c; 2\times8g$	$4d; 4\times8g$	$4e; 4\times8g$	$4f; 4\times8g$	$9\times8g$
[p^2] $P4/n$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$; p = prime $= 4n-1$; $u, v = 1, \dots, p-1$		$2a$; $\frac{p^2-1}{4}\times8g$	$2b$; $\frac{p^2-1}{4}\times8g$	$2c$; $\frac{p^2-1}{4}\times8g$	$4d$; $\frac{p^2-1}{2}\times8g$	$4e$; $\frac{p^2-1}{2}\times8g$	$4f$; $\frac{p^2-1}{2}\times8g$	$p^2\times8g$

C_{4h}^{4} No. 86 $P4_2/n$

	Axes	Coordinates origin 1	Coordinates origin 2	2a	2b	4c	4d	4e	4f	8g
I Maximal *translationengleiche* subgroups										
[2] $P4_2$ (77)		$x+\frac{1}{2},y,z$	$x+\frac{1}{4},y-\frac{1}{4},z$	$2c$	$2c$	$4d$	$4d$	$2a;2b$	$2\times2c$	$2\times4d$
[2] $P\bar{4}$ (81)			$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$1a;1d$	$1b;1c$	$4h$	$4h$	$2\times2g$	$2e;2f$	$2\times4h$
[2] $P112/n$ (13)		$x-\frac{1}{4},y-\frac{1}{4},z-\frac{1}{4}$		$2e$	$2e$	$2a;2b$	$2c;2d$	$2\times2f$	$2\times2e$	$2\times4g$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $I4_1/a$ (88)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),\frac{1}{2}z;\ +(0,0,\frac{1}{2})$		$4a;4b$	$8e$	$8c;8d$	$16f$	$16f$	$2\times8e$	$2\times16f$
[2] $I4_1/a$ (88)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$		$8e$	$4a;4b$	$16f$	$8c;8d$	$16f$	$2\times8e$	$2\times16f$
[2] $I4_1/a$ (88)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),\frac{1}{2}z;\ +(0,0,\frac{1}{2})$		$8e$	$4a;4b$	$8c;8d$	$16f$	$16f$	$2\times8e$	$2\times16f$
[2] $I4_1/a$ (88)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$		$4a;4b$	$8e$	$16f$	$8c;8d$	$16f$	$2\times8e$	$2\times16f$
Enlarged unit cell, isomorphic										
[3] $P4_2/n$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a(b^*);4f$	$2b(a^*);4f$	$4d(c^*);8g$	$4c(d^*);8g$	$3\times4e$	$3\times4f$	$3\times8g$
[p] $P4_2/n$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$2a(b^\dagger)$; $\frac{p-1}{2}\times4f$	$2b(a^\dagger)$; $\frac{p-1}{2}\times4f$	$4c(d^\ddagger)$; $\frac{p-1}{2}\times8g$	$4d(c^\ddagger)$; $\frac{p-1}{2}\times8g$	$p\times4e$	$p\times4f$	$p\times8g$
	$p=\text{prime}>2;\ u=1,\ldots,p-1$									
[5] $P4_2/n$	$\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z;$	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z;$	$2a(b^*);8g$	$2b(a^*);8g$	$4c;2\times8g$	$4d;2\times8g$	$4e;2\times8g$	$4f;2\times8g$	$5\times8g$
		$\pm(\frac{1}{5},\frac{3}{5},0);\ \pm(\frac{2}{5},\frac{1}{5},0)$								
[5] $P4_2/n$	$\mathbf{a}-2\mathbf{b}$, $2\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z;$	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z;$	$2a(b^*);8g$	$2b(a^*);8g$	$4c;2\times8g$	$4d;2\times8g$	$4e;2\times8g$	$4f;2\times8g$	$5\times8g$
		$\pm(\frac{1}{5},\frac{2}{5},0);\ \pm(\frac{3}{5},\frac{1}{5},0)$								
[p] $P4_2/n$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z;\ +(\frac{uq}{p},\frac{ur}{p},0)$	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z;\ +(\frac{uq}{p},\frac{ur}{p},0)$	$2a(b^{**})$; $\frac{p-1}{4}\times8g$	$2b(a^{**})$; $\frac{p-1}{4}\times8g$	$4c$; $\frac{p-1}{2}\times8g$	$4d$; $\frac{p-1}{2}\times8g$	$4e$; $\frac{p-1}{2}\times8g$	$4f$; $\frac{p-1}{2}\times8g$	$p\times8g$
	$p=q^2+r^2=\text{prime}=4n+1;$ $q=2n+1\geq1;\ r=\pm2n'\neq0;\ u=1,\ldots,p-1$									
[9] $P4_2/n$	$3\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$	$\frac{1}{3}x,\frac{1}{3}y,z;$	$2a(b^*)$; $2\times8g$	$2b(a^*)$; $2\times8g$	$4c;4\times8g$	$4d;4\times8g$	$4e;4\times8g$	$4f;4\times8g$	$9\times8g$
		$\pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$								
[p^2] $P4_2/n$	$p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$2a(b^\dagger)$; $\frac{p^2-1}{4}\times8g$	$2b(a^\dagger)$; $\frac{p^2-1}{4}\times8g$	$4c$; $\frac{p^2-1}{2}\times8g$	$4d$; $\frac{p^2-1}{2}\times8g$	$4e$; $\frac{p^2-1}{2}\times8g$	$4f$; $\frac{p^2-1}{2}\times8g$	$p^2\times8g$
	$p=\text{prime}=4n-1;\ u,v=1,\ldots,p-1$									

* origin 2

† origin 2 and $p=4n-1$

‡ origin 1 and $p=4n-1$

** origin 2 and $q+r=4n-1$

$I4/m$ No. 87 C_{4h}^5

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$4c$	$4d$ $8g$	$4e$ $8h$	$8f$ $16i$
I Maximal *translationengleiche* subgroups								
[2] $I\bar{4}$ (82)			$2a$	$2b$	$4f$	$2c;2d$ $2\times4f$	$4e$ $8g$	$8g$ $2\times8g$
[2] $I4$ (79)			$2a$	$2a$	$4b$	$4b$ $2\times4b$	$2\times2a$ $8c$	$8c$ $2\times8c$
[2] $I112/m$ (12)			$2a$	$2b$	$2c;2d$	$4h$ $2\times4h$	$4g$ $2\times4i$	$4e;4f$ $2\times8j$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P4_2/n$ (86)		origin 1: x,y,z origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$2a$	$2b$	$4e$	$4e$ $2\times4e$	$4f$ $8g$	$4c;4d$ $2\times8g$
[2] $P4/n$ (85)		origin 1: $x+\frac{1}{2},y,z+\frac{1}{4}$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$2c$	$2c$	$4f$	$2a;2b$ $2\times4f$	$2\times2c$ $8g$	$4d;4e$ $2\times8g$
[2] $P4_2/m$ (84)		$x+\frac{1}{2},y,z$	$2d$	$2c$	$2a;2b$	$2e;2f$ $4g;4h$	$4i$ $2\times4j$	$8k$ $2\times8k$
[2] $P4/m$ (83)			$1a;1d$	$1b;1c$	$2e;2f$	$4i$ $2\times4i$	$2g;2h$ $4j;4k$	$8l$ $2\times8l$
Enlarged unit cell, isomorphic								
[3] $I4/m$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$4c;8g$	$4d;8g$ $3\times8g$	$3\times4e$ $8h;16i$	$8f;16i$ $3\times16i$
[p] $I4/m$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=\text{prime}>2;\ u=1,\dots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$4c;\frac{p-1}{2}\times8g$	$4d;\frac{p-1}{2}\times8g$ $p\times8g$	$p\times4e$ $8h;\frac{p-1}{2}\times16i$	$8f;\frac{p-1}{2}\times16i$ $p\times16i$
[5] $I4/m$	$\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{5}(x+2y),\frac{1}{5}(-2x+y),z;$ $\pm(\frac{1}{5},\frac{3}{5},0);\ \pm(\frac{2}{5},\frac{1}{5},0)$	$2a;8h$	$2b;8h$	$4c;2\times8h$	$4d;16i$ $8g;2\times16i$	$4e;16i$ $5\times8h$	$8f;2\times16i$ $5\times16i$
[5] $I4/m$	$\mathbf{a}-2\mathbf{b}$, $2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{5}(x-2y),\frac{1}{5}(2x+y),z;$ $\pm(\frac{1}{5},\frac{2}{5},0);\ \pm(\frac{3}{5},\frac{1}{5},0)$	$2a;8h$	$2b;8h$	$4c;2\times8h$	$4d;16i$ $8g;2\times16i$	$4e;16i$ $5\times8h$	$8f;2\times16i$ $5\times16i$
[p] $I4/m$	$q\mathbf{a}-r\mathbf{b}$, $r\mathbf{a}+q\mathbf{b},\mathbf{c}$ $p=q^2+r^2=\text{prime}=4n+1;$ $q=2n+1\geq1;\ r=\pm2n'\neq0;$	$\frac{1}{p}(qx-ry),\frac{1}{p}(rx+qy),z;$ $+(\frac{uq}{p},\frac{ur}{p},0)$ $u=1,\dots,p-1$	$2a;\frac{p-1}{4}\times8h$	$2b;\frac{p-1}{4}\times8h$	$4c;\frac{p-1}{2}\times8h$	$4d;\frac{p-1}{4}\times16i$ $8g;\frac{p-1}{2}\times16i$	$4e;\frac{p-1}{4}\times16i$ $p\times8h$	$8f;\frac{p-1}{2}\times16i$ $p\times16i$
[9] $I4/m$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times8h$	$2b;2\times8h$	$4c;4\times8h$	$4d;2\times16i$ $8g;4\times16i$	$4e;2\times16i$ $9\times8h$	$8f;4\times16i$ $9\times16i$
[p^2] $I4/m$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=\text{prime}=4n-1;$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\dots,p-1$	$2a;\frac{p^2-1}{4}\times8h$	$2b;\frac{p^2-1}{4}\times8h$	$4c;\frac{p^2-1}{2}\times8h$	$4d;\frac{p^2-1}{4}\times16i$ $8g;\frac{p^2-1}{2}\times16i$	$4e;\frac{p^2-1}{4}\times16i$ $p^2\times8h$	$8f;\frac{p^2-1}{2}\times16i$ $p^2\times16i$

C_{4h}^{6} No. 88 $I4_1/a$

	Axes	Coordinates origin 1	 origin 2	Wyckoff positions $4a$	 $4b$	 $8c$	 $8d$	 $8e$	 $16f$
I Maximal *translationengleiche* subgroups									
[2] $I\bar{4}$ (82)			$x,y+\frac{1}{4},z+\frac{1}{8}$	$2a;2c$	$2b;2d$	$8g$	$8g$	$4e;4f$	$2\times 8g$
[2] $I4_1$ (80)			$x,y+\frac{1}{4},z$	$4a$	$4a$	$8b$	$8b$	$2\times 4a$	$2\times 8b$
[2] $I112/b$ (15) $\widehat{=} A112/a$	 **b**, −**a**−**b**, **c**	$x,y-\frac{1}{4},z-\frac{1}{8}$ $-x+y-\frac{1}{4},-x,z-\frac{1}{8}$	 $-x+y,-x,z$	$4e$	$4e$	$4a;4d$	$4b;4c$	$2\times 4e$	$2\times 8f$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**									
[3] $I4_1/a$	**a**, **b**, 3**c**	$x+\frac{1}{2},y,\frac{1}{3}z-\frac{1}{4}$; $\pm(0,0,\frac{1}{3})$	$x+\frac{1}{2},y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a;8e$	$4b;8e$	$8d;16f$	$8c;16f$	$3\times 8e$	$3\times 16f$
[5] $I4_1/a$	**a**, **b**, 5**c**	$x,y,\frac{1}{5}z$; $\pm(0,0,\frac{1}{5});\pm(0,0,\frac{2}{5})$	$x,y,\frac{1}{5}z$;	$4a(b^*);2\times 8e$	$4b(a^*);2\times 8e$	$8d(c^*)$; $2\times 16f$	$8c(d^*)$; $2\times 16f$	$5\times 8e$	$5\times 16f$
[p] $I4_1/a$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime $=4n+1$; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$4a(b^\dagger)$; $\frac{p-1}{2}\times 8e$	$4b(a^\dagger)$; $\frac{p-1}{2}\times 8e$	$8c(d^{\dagger\dagger})$ $\frac{p-1}{2}\times 16f$	$8d(c^{\dagger\dagger})$; $\frac{p-1}{2}\times 16f$	$p\times 8e$	$p\times 16f$
[p] $I4_1/a$	**a**, **b**, p**c**	$x+\frac{1}{2},y,\frac{1}{p}z-\frac{1}{4}$; $+(0,0,\frac{u}{p})$ p = prime $=4n-1$; $u=1,\ldots,p-1$	$x+\frac{1}{2},y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$4a(b^\ddagger)$; $\frac{p-1}{2}\times 8e$	$4b(a^\ddagger)$; $\frac{p-1}{2}\times 8e$	$8d(c^{\ddagger\ddagger})$; $\frac{p-1}{2}\times 16f$	$8c(d^{\ddagger\ddagger})$; $\frac{p-1}{2}\times 16f$	$p\times 8e$	$p\times 16f$
[5] $I4_1/a$	**a**+2**b**, −2**a**+**b**, **c**	$\frac{1}{5}(x+2y)$, $\frac{1}{5}(-2x+y),z$; $\pm(\frac{1}{5},\frac{3}{5},0);\pm(\frac{2}{5},\frac{1}{5},0)$	$\frac{1}{5}(x+2y)+\frac{1}{2}$, $\frac{1}{5}(-2x+y),z$;	$4a;16f$	$4b;16f$	$8d;2\times 16f$	$8c;2\times 16f$	$8e;2\times 16f$	$5\times 16f$
[5] $I4_1/a$	**a**−2**b**, 2**a**+**b**, **c**	$\frac{1}{5}(x-2y)$, $\frac{1}{5}(2x+y),z$; $\pm(\frac{1}{5},\frac{2}{5},0);\pm(\frac{3}{5},\frac{1}{5},0)$	$\frac{1}{5}(x-2y)+\frac{1}{2}$, $\frac{1}{5}(2x+y),z$;	$4a;16f$	$4b;16f$	$8d;2\times 16f$	$8c;2\times 16f$	$8e;2\times 16f$	$5\times 16f$
[p] $I4_1/a$	q**a**−r**b**, r**a**+q**b**, **c**	$\frac{1}{p}(qx-ry)$, $\frac{1}{p}(rx+qy),z$; $+(\frac{uq}{p},\frac{ur}{p},0)$ $p=q^2+r^2$ = prime $=4n+1$; $q=2n+1\geq 1$; $r=\pm 4n'\neq 0$; $u=1,\ldots,p-1$ $s=0$ if $q=4n+1$; $s=\frac{1}{2}$ if $q=4n-1$	$\frac{1}{p}(qx-ry)$, $\frac{1}{p}(rx+qy)+s,z$; $+(\frac{uq}{p},\frac{ur}{p},0)$	$4a;\frac{p-1}{4}\times 16f$	$4b;\frac{p-1}{4}\times 16f$	$8c$; $\frac{p-1}{2}\times 16f$	$8d$; $\frac{p-1}{2}\times 16f$	$8e$; $\frac{p-1}{2}\times 16f$	$p\times 16f$
[p] $I4_1/a$	q**a**−r**b**, r**a**+q**b**, **c**	$\frac{1}{p}(qx-ry)$, $\frac{1}{p}(rx+qy),z$; $+(\frac{uq}{p},\frac{ur}{p},0)$ $p=q^2+r^2$ = prime $=4n+1$; $q=2n+1\geq 1$; $r=\pm 4n'+2$; $u=1,\ldots,p-1$ $s=0$ if $q=4n+1$; $s=\frac{1}{2}$ if $q=4n-1$	$\frac{1}{p}(qx-ry)+\frac{1}{2}$, $\frac{1}{p}(rx+qy)+s,z$; $+(\frac{uq}{p},\frac{ur}{p},0)$	$4a;\frac{p-1}{4}\times 16f$	$4b;\frac{p-1}{4}\times 16f$	$8d$; $\frac{p-1}{2}\times 16f$	$8c$; $\frac{p-1}{2}\times 16f$	$8e$; $\frac{p-1}{2}\times 16f$	$p\times 16f$
[9] $I4_1/a$	3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z$; $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$\frac{1}{3}x,\frac{1}{3}y+\frac{1}{2},z$;	$4a;2\times 16f$	$4b;2\times 16f$	$8c;4\times 16f$	$8d;4\times 16f$	$8e;4\times 16f$	$9\times 16f$
[p^2] $I4_1/a$	p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$ p = prime $=4n-1$; $u,v=1,\ldots,p-1$ $s=0$ if $p=4n+1$; $s=\frac{1}{2}$ if $p=4n-1$	$\frac{1}{p}x,\frac{1}{p}y+s,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$4a;\frac{p^2-1}{4}\times 16f$	$4b;\frac{p^2-1}{4}\times 16f$	$8c$; $\frac{p^2-1}{2}\times 16f$	$8d$; $\frac{p^2-1}{2}\times 16f$	$8e$; $\frac{p^2-1}{2}\times 16f$	$p^2\times 16f$

* origin 2
† origin 2 and $p=8n+5$ †† origin 1 and $p=8n+5$
‡ origin 2 and $p=8n-1$ ‡‡ origin 1 and $p=8n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 89, pp. 564–565.

$P422$ No. 89 D_4^1

	Axes	Coordinates	Wyckoff positions 1a	 1b	 1c	 1d	 2e	 2f	 2g 4l	 2h 4m	 4i 4n	 4j 4o	 4k 8p
I Maximal *translationengleiche* subgroups													
[2] $P4$ (75)			1a	1a	1b	1b	2c	2c	2×1a 4d	2×1b 4d	2×2c 4d	4d 4d	4d 2×4d
[2] $P222$ (16)			1a	1d	1e	1h	1b; 1c	1f; 1g	2q 2i; 2m	2t 2l; 2p	2r; 2s 2j; 2n	4u 2k; 2o	4u 2×4u
[2] $C222$ (21)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	2a	2d	2b	2c	4k	4k	4i 8l	4j 8l	2×4k 8l	4e; 4g 8l	4f; 4h 2×8l
II Maximal *klassengleiche* subgroups													
Enlarged unit cell, non-isomorphic													
[2] $I422$ (97)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	2a; 2b	4e	4c	4d	8g	8j	2×4e 2×8g	8f 2×8j	16k 16k	8h; 8i 16k	16k 2×16k
[2] $I422$ (97)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z; +(0,0,\frac{1}{2})$	4c	4d	2a; 2b	4e	8g	8j	8f 16k	2×4e 16k	16k 2×8j	8h; 8i 2×8g	16k 2×16k
[2] $I422$ (97)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	4e	2a; 2b	4d	4c	8j	8g	2×4e 16k	8f 16k	16k 2×8g	16k 2×8j	8h; 8i 2×16k
[2] $I422$ (97)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	4d	4c	4e	2a; 2b	8j	8g	8f 2×8j	2×4e 2×8g	16k 16k	16k 16k	8h; 8i 2×16k
[2] $P4_222$ (93)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2a	2e	2b	2f	2c; 2d	4i	4g 4j; 4l	4h 8p	2×4i 8p	8p 4k; 4m	4n; 4o 2×8p
[2] $P4_222$ (93)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	2e	2a	2f	2b	4i	2c; 2d	4g 8p	4h 4k; 4m	2×4i 4j; 4l	4n; 4o 8p	8p 2×8p
[2] $P42_12$ (90)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	2a	2b	2c	2c	4e	4f	4d 2×4e	2×2c 8g	8g 2×4f	8g 8g	8g 2×8g
[2] $P42_12$ (90)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	2c	2c	2a	2b	4e	4f	2×2c 8g	4d 2×4f	8g 8g	8g 2×4e	8g 2×8g
Enlarged unit cell, isomorphic													
[2] $P422$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	1a; 1b	2g	1c; 1d	2h	2e; 2f	4i	2×2g 4l; 4n	2×2h 8p	2×4i 8p	4j; 4k 4m; 4o	8p 2×8p
[2] $P422$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	2g	1a; 1b	2h	1c; 1d	4i	2e; 2f	2×2g 8p	2×2h 4m; 4o	2×4i 4l; 4n	8p 8p	4j; 4k 2×8p
[3] $P422$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	1a; 2g	1b; 2g	1c; 2h	1d; 2h	2e; 4i	2f; 4i	3×2g 4l; 8p	3×2h 4m; 8p	3×4i 4n; 8p	4j; 8p 4o; 8p	4k; 8p 3×8p

	Axes	Coordinates	Wyckoff positions: $1a$	$1b$ $2h$	$1c$ $4i$	$1d$ $4j$	$2e$ $4k$ $4n$	$2f$ $4l$ $4o$	$2g$ $4m$ $8p$
$[p]\ P422$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$ $p = \text{prime} > 2$; $u = 1, \ldots, p-1$	$1a; \frac{p-1}{2}\times 2g$	$1b; \frac{p-1}{2}\times 2g$ $p\times 2h$	$1c; \frac{p-1}{2}\times 2h$ $p\times 4i$	$1d; \frac{p-1}{2}\times 2h$ $4j; \frac{p-1}{2}\times 8p$	$2e; \frac{p-1}{2}\times 4i$ $4k; \frac{p-1}{2}\times 8p$ $4n; \frac{p-1}{2}\times 8p$	$2f; \frac{p-1}{2}\times 4i$ $4l; \frac{p-1}{2}\times 8p$ $4o; \frac{p-1}{2}\times 8p$	$p\times 2g$ $4m; \frac{p-1}{2}\times 8p$ $p\times 8p$
$[2]\ P422$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z$; $+(\frac{1}{2}, \frac{1}{2}, 0)$	$1a; 1c$	$1b; 1d$ $4i$	$2e$ $8p$	$2f$ $4l; 4o$	$4j$ $4m; 4n$ $2\times 4k$	$4k$ $2\times 4j$ $8p$	$2g; 2h$ $8p$ $2\times 8p$
$[2]\ P422$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y), z$; $+(\frac{1}{2}, \frac{1}{2}, 0)$	$2e$	$2f$ $2g; 2h$	$1a; 1c$ $8p$	$1b; 1d$ $4l; 4o$	$4j$ $4m; 4n$ $8p$	$4k$ $8p$ $2\times 4j$	$4i$ $2\times 4k$ $2\times 8p$
$[9]\ P422$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3}, 0, 0)$; $\pm(0, \frac{1}{3}, 0)$; $\pm(\frac{1}{3}, \frac{1}{3}, 0)$; $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	$1a; 4j; 4l$	$1b; 4k; 4n$ $2h; 2\times 8p$	$1c; 4j; 4o$ $4i; 4\times 8p$	$1d; 4k; 4m$ $3\times 4j; 3\times 8p$	$2e; 4l; 4o; 8p$ $3\times 4k; 3\times 8p$ $3\times 4n; 3\times 8p$	$2f; 4m; 4n; 8p$ $3\times 4l; 3\times 8p$ $3\times 4o; 3\times 8p$	$2g; 2\times 8p$ $3\times 4m; 3\times 8p$ $9\times 8p$
$[p^2]\ P422$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$ $p = \text{prime} > 2$; $u, v = 1, \ldots, p-1$	$1a; \frac{p-1}{2}\times 4j$; $\frac{p-1}{2}\times 4l$; $\frac{(p-1)(p-3)}{8}\times 8p$	$1b; \frac{p-1}{2}\times 4k$; $\frac{p-1}{2}\times 4n$; $\frac{(p-1)(p-3)}{8}\times 8p$ $2h; \frac{p^2-1}{4}\times 8p$	$1c; \frac{p-1}{2}\times 4j$; $\frac{p-1}{2}\times 4o$; $\frac{(p-1)(p-3)}{8}\times 8p$ $4i; \frac{p^2-1}{2}\times 8p$	$1d; \frac{p-1}{2}\times 4k$; $\frac{p-1}{2}\times 4m$; $\frac{(p-1)(p-3)}{8}\times 8p$ $p\times 4j$; $\frac{p(p-1)}{2}\times 8p$	$2e; \frac{p-1}{2}\times 4l$; $\frac{p-1}{2}\times 4o$; $\frac{(p-1)^2}{4}\times 8p$ $p\times 4k$; $\frac{p(p-1)}{2}\times 8p$ $p\times 4n$; $\frac{p(p-1)}{2}\times 8p$	$2f; \frac{p-1}{2}\times 4m$; $\frac{p-1}{2}\times 4n$; $\frac{(p-1)^2}{4}\times 8p$ $p\times 4l$; $\frac{p(p-1)}{2}\times 8p$ $p\times 4o$; $\frac{p(p-1)}{2}\times 8p$	$2g; \frac{p^2-1}{4}\times 8p$ $p\times 4m$; $\frac{p(p-1)}{2}\times 8p$ $p^2\times 8p$

$P42_12$ No. 90 D_4^2

	Axes	Coordinates	Wyckoff positions $2a$	$2b$	$2c$	$4d$	$4e$	$4f$	$8g$
I Maximal *translationengleiche* subgroups									
[2] $P4$ (75)		$x+\frac{1}{2},y,z$	$2c$	$2c$	$1a;1b$	$2\times2c$	$4d$	$4d$	$2\times4d$
[2] $P2_12_12$ (18)			$2a$	$2a$	$2b$	$2\times2a$	$4c$	$4c$	$2\times4c$
[2] $C222$ (21)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$2a;2b$	$2c;2d$	$4k$	$4i;4j$	$4e;4g$	$4f;4h$	$2\times8l$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $P4_22_12$ (94)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2a;2b$	$4c$	$4d$	$2\times4c$	$4e;4f$	$8g$	$2\times8g$
[2] $P4_22_12$ (94)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4c$	$2a;2b$	$4d$	$2\times4c$	$8g$	$4e;4f$	$2\times8g$
Enlarged unit cell, isomorphic									
[2] $P42_12$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2a;2b$	$4d$	$2\times2c$	$2\times4d$	$4e;4f$	$8g$	$2\times8g$
[2] $P42_12$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4d$	$2a;2b$	$2\times2c$	$2\times4d$	$8g$	$4e;4f$	$2\times8g$
[3] $P42_12$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4d$	$2b;4d$	$3\times2c$	$3\times4d$	$4e;8g$	$4f;8g$	$3\times8g$
[p] $P42_12$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=\text{prime}>2$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4d$	$2b;\frac{p-1}{2}\times4d$	$p\times2c$	$p\times4d$	$4e;\frac{p-1}{2}\times8g$	$4f;\frac{p-1}{2}\times8g$	$p\times8g$
[9] $P42_12$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times4e;8g$	$2b;2\times4f;8g$	$2c;2\times8g$	$4d;4\times8g$	$3\times4e;3\times8g$	$3\times4f;3\times8g$	$9\times8g$
[p^2] $P42_12$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=\text{prime}>2;$	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a;(p-1)\times4e;$ $\frac{(p-1)^2}{4}\times8g$	$2b;(p-1)\times4f;$ $\frac{(p-1)^2}{4}\times8g$	$2c;$ $\frac{p^2-1}{4}\times8g$	$4d;$ $\frac{p^2-1}{2}\times8g$	$p\times4e;$ $\frac{p(p-1)}{2}\times8g$	$p\times4f;$ $\frac{p(p-1)}{2}\times8g$	$p^2\times8g$

D_4^3 No. 91 $P4_122$

	Axes	Coordinates	Wyckoff positions 4a	4b	4c	8d
I Maximal *translationengleiche* subgroups						
[2] $P4_1$ (76)			$4a$	$4a$	$4a$	$2\times4a$
[2] $P222_1$ (17)		$x,y,z+\frac{1}{4}$	$2a;2c$	$2b;2d$	$4e$	$2\times4e$
[2] $C222_1$ (20)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y),\frac{1}{2}(-x+y),z+\frac{1}{8}$	$8c$	$8c$	$4a;4b$	$2\times8c$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $P4_12_12$ (92)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y),\frac{1}{2}(-x+y),z;\ +(\frac{1}{2},\frac{1}{2},0)$	$2\times4a$	$8b$	$8b$	$2\times8b$
[2] $P4_12_12$ (92)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{2},\frac{1}{2}(-x+y),z;\ +(\frac{1}{2},\frac{1}{2},0)$	$8b$	$2\times4a$	$8b$	$2\times8b$
Enlarged unit cell, isomorphic						
[3] $P4_322$ (95)	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$4a;8d$	$4b;8d$	$4c;8d$	$3\times8d$
[p] $P4_322$ (95)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$4a;\ \frac{p-1}{2}\times8d$	$4b;\ \frac{p-1}{2}\times8d$	$4c;\ \frac{p-1}{2}\times8d$	$p\times8d$
	$p = \text{prime} = 4n-1;\ u=1,\ldots,p-1$					
[5] $P4_122$	$\mathbf{a},\mathbf{b},5\mathbf{c}$	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});\ \pm(0,0,\frac{2}{5})$	$4a;2\times8d$	$4b;2\times8d$	$4c;2\times8d$	$5\times8d$
[p] $P4_122$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$4a;\ \frac{p-1}{2}\times8d$	$4b;\ \frac{p-1}{2}\times8d$	$4c;\ \frac{p-1}{2}\times8d$	$p\times8d$
	$p = \text{prime} = 4n+1;\ u=1,\ldots,p-1$					
[2] $P4_122$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y),\frac{1}{2}(-x+y),z-\frac{1}{8};\ +(\frac{1}{2},\frac{1}{2},0)$	$2\times4c$	$8d$	$4a;4b$	$2\times8d$
[2] $P4_122$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{2},\frac{1}{2}(-x+y),z-\frac{1}{8};\ +(\frac{1}{2},\frac{1}{2},0)$	$8d$	$2\times4c$	$4a;4b$	$2\times8d$
[9] $P4_122$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;\ \pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$	$3\times4a;3\times8d$	$3\times4b;3\times8d$	$3\times4c;3\times8d$	$9\times8d$
[p^2] $P4_122$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$p\times4a;$ $\frac{p(p-1)}{2}\times8d$	$p\times4b;$ $\frac{p(p-1)}{2}\times8d$	$p\times4c;$ $\frac{p(p-1)}{2}\times8d$	$p^2\times8d$
	$p = \text{prime} > 2;\ u,v=1,\ldots,p-1$					

$P4_12_12$ No. 92 D_4^4

	Axes	Coordinates	Wyckoff positions $4a$	$8b$
I Maximal *translationengleiche* subgroups				
[2] $P4_1$ (76)		$x+\frac{1}{2},y,z$	$4a$	$2\times4a$
[2] $P2_12_12_1$ (19)		$x+\frac{1}{4},y,z+\frac{1}{8}$	$4a$	$2\times4a$
[2] $C222_1$ (20)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y),\frac{1}{2}(-x+y),z$	$4a;4b$	$2\times8c$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**				
[3] $P4_32_12$ (96)	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$4a;8b$	$3\times8b$
[p] $P4_32_12$ (96)	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}=4n-1;\ u=1,\ldots,p-1$	$4a;\ \frac{p-1}{2}\times8b$	$p\times8b$
[5] $P4_12_12$	$\mathbf{a},\mathbf{b},5\mathbf{c}$	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});\ \pm(0,0,\frac{2}{5})$	$4a;2\times8b$	$5\times8b$
[p] $P4_12_12$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}=4n+1;\ u=1,\ldots,p-1$	$4a;\ \frac{p-1}{2}\times8b$	$p\times8b$
[9] $P4_12_12$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;\ \pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$	$3\times4a;3\times8b$	$9\times8b$
[p^2] $P4_12_12$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>2;\ u,v=1,\ldots,p-1$	$p\times4a;\frac{p(p-1)}{2}\times8b$	$p^2\times8b$

$P4_222$ No. 93

CONTINUED (*from next page*)

	Axes, Coordinates	Wyckoff positions $1a$ $2g$	$1b$ $2h$	$1c$ $4i$ $4m$	$1d$ $4j$ $4n$	$2e$ $4k$ $4o$	$2f$ $4l$ $8p$
[p] $P4_222$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}>2;$ $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4g$ $p\times4g$	$2b;\frac{p-1}{2}\times4h$ $p\times4h$	$2c;\frac{p-1}{2}\times4i$ $p\times4i$ $4m;\frac{p-1}{2}\times8p$	$2d;\frac{p-1}{2}\times4i$ $4j;\frac{p-1}{2}\times8p$ $4n(o^*);\ \frac{p-1}{2}\times8p$	$2e;\frac{p-1}{2}\times4g$ $4k;\frac{p-1}{2}\times8p$ $4o(n^*);\ \frac{p-1}{2}\times8p$	$2f;\frac{p-1}{2}\times4h$ $4l;\frac{p-1}{2}\times8p$ $p\times8p$
[2] $P4_222$	$\mathbf{a}-\mathbf{b}$, $\frac{1}{2}(x-y),\frac{1}{2}(x+y),$ $\mathbf{a}+\mathbf{b},\mathbf{c}$ $z+\frac{1}{4};\ +(\frac{1}{2},\frac{1}{2},0)$	$2e;2f$ $4g;4h$	$4i$ $2\times4i$	$4o$ $8p$ $8p$	$4n$ $2\times4n$ $4j;4m$	$2a;2b$ $8p$ $4k;4l$	$2c;2d$ $2\times4o$ $2\times8p$
[2] $P4_222$	$\mathbf{a}-\mathbf{b}$, $\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),$ $\mathbf{a}+\mathbf{b},\mathbf{c}$ $z+\frac{1}{4};\ +(\frac{1}{2},\frac{1}{2},0)$	$4i$ $2\times4i$	$2e;2f$ $4g;4h$	$4n$ $8p$ $2\times4n$	$4o$ $8p$ $4j;4m$	$2c;2d$ $2\times4o$ $4k;4l$	$2a;2b$ $8p$ $2\times8p$
[9] $P4_222$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$ $\frac{1}{3}x,\frac{1}{3}y,z;\ \pm(\frac{1}{3},0,0);$ $\pm(0,\frac{1}{3},0);\pm(\frac{1}{3},\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4j;4l;8p$ $4g;4\times8p$	$2b;4k;4m;8p$ $4h;4\times8p$	$2c;4l;4m;8p$ $4i;4\times8p$ $3\times4m;3\times8p$	$2d;4j;4k;8p$ $3\times4j;3\times8p$ $3\times4n;3\times8p$	$2e;4n;4o;8p$ $3\times4k;3\times8p$ $3\times4o;3\times8p$	$2f;4n;4o;8p$ $3\times4l;3\times8p$ $9\times8p$
[p^2] $P4_222$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ $\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>2;$ $u,v=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4j;$ $\frac{p-1}{2}\times4l;$ $\frac{(p-1)^2}{4}\times8p$ $4g;\ \frac{p^2-1}{2}\times8p$	$2b;\frac{p-1}{2}\times4k;$ $\frac{p-1}{2}\times4m;$ $\frac{(p-1)^2}{4}\times8p$ $4h;\frac{p^2-1}{2}\times8p$	$2c;\frac{p-1}{2}\times4l;$ $\frac{p-1}{2}\times4m;$ $\frac{(p-1)^2}{4}\times8p$ $4i;\frac{p^2-1}{2}\times8p$ $p\times4m;$ $\frac{p(p-1)}{2}\times8p$	$2d;\frac{p-1}{2}\times4j;$ $\frac{p-1}{2}\times4k;$ $\frac{(p-1)^2}{4}\times8p$ $p\times4j;$ $\frac{p(p-1)}{2}\times8p$ $p\times4n;$ $\frac{p(p-1)}{2}\times8p$	$2e;\frac{p-1}{2}\times4n;$ $\frac{p-1}{2}\times4o;$ $\frac{(p-1)^2}{4}\times8p$ $p\times4k;$ $\frac{p(p-1)}{2}\times8p$ $p\times4o;$ $\frac{p(p-1)}{2}\times8p$	$2f;\frac{p-1}{2}\times4n;$ $\frac{p-1}{2}\times4o;$ $\frac{(p-1)^2}{4}\times8p$ $p\times4l;$ $\frac{p(p-1)}{2}\times8p$ $p^2\times8p$

$^*\ p=4n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 93, pp. 568–569.

D_4^5 No. 93 $P4_222$

	Axes	Coordinates	Wyckoff positions $2a$	$2b$	$2c$	$2d$	$2e$	$2f$	$4g$ $4l$	$4h$ $4m$	$4i$ $4n$	$4j$ $4o$	$4k$ $8p$
I Maximal *translationengleiche* subgroups													
[2] $P4_2$ (77)			$2a$	$2b$	$2c$	$2c$	$2a$	$2b$	$2\times2a$ $4d$	$2\times2b$ $4d$	$2\times2c$ $4d$	$4d$ $4d$	$4d$ $2\times4d$
[2] $P222$ (16)			$1a;1d$	$1e;1h$	$1c;1f$	$1b;1g$	$2q$	$2t$	$2\times2q$ $2j;2m$	$2\times2t$ $2k;2p$	$2r;2s$ $4u$	$2i;2n$ $4u$	$2l;2o$ $2\times4u$
[2] $C222$ (21)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x{-}y),\frac{1}{2}(x{+}y),z{+}\frac{1}{4}$	$4i$	$4j$	$4k$	$4k$	$2a;2d$	$2b;2c$	$2\times4i$ $8l$	$2\times4j$ $8l$	$2\times4k$ $4e;4h$	$8l$ $4f;4g$	$8l$ $2\times8l$
II Maximal *klassengleiche* subgroups													
Enlarged unit cell, non-isomorphic													
[2] $I4_122$ (98)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x{-}y){+}\frac{1}{4},\frac{1}{2}(x{+}y){+}\frac{1}{4},\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$8d$	$8e$	$8c$	$4a;4b$	$8f$	$8f$	$16g$ $16g$	$16g$ $16g$	$2\times8c$ $16g$	$2\times8d$ $2\times8f$	$2\times8e$ $2\times16g$
[2] $I4_122$ (98)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x{-}y){-}\frac{1}{4},\frac{1}{2}(x{+}y){+}\frac{1}{4},\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$8e$	$8d$	$4a;4b$	$8c$	$8f$	$8f$	$16g$ $2\times8e$	$16g$ $2\times8d$	$2\times8c$ $16g$	$16g$ $2\times8f$	$16g$ $2\times16g$
[2] $I4_122$ (98)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x{-}y){+}\frac{1}{4},\frac{1}{2}(x{+}y){+}\frac{1}{4},\frac{1}{2}z{+}\frac{1}{4};\ +(0,0,\frac{1}{2})$	$8d$	$8e$	$4a;4b$	$8c$	$8f$	$8f$	$16g$ $2\times8d$	$16g$ $2\times8e$	$2\times8c$ $2\times8f$	$16g$ $16g$	$16g$ $2\times16g$
[2] $I4_122$ (98)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x{-}y){-}\frac{1}{4},\frac{1}{2}(x{+}y){+}\frac{1}{4},\frac{1}{2}z{+}\frac{1}{4};\ +(0,0,\frac{1}{2})$	$8e$	$8d$	$8c$	$4a;4b$	$8f$	$8f$	$16g$ $16g$	$16g$ $16g$	$2\times8c$ $2\times8f$	$2\times8e$ $16g$	$2\times8d$ $2\times16g$
[2] $P4_322$ (95)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4b$	$4a$	$4b$	$4c$	$4c$	$8d$ $2\times4a$	$8d$ $8d$	$8d$ $2\times4c$	$8d$ $8d$	$2\times4b$ $2\times8d$
[2] $P4_322$ (95)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z{+}\frac{1}{4};{+}(0,0,\frac{1}{2})$	$4a$	$4b$	$4b$	$4a$	$4c$	$4c$	$8d$ $8d$	$8d$ $2\times4b$	$8d$ $8d$	$2\times4a$ $2\times4c$	$8d$ $2\times8d$
[2] $P4_22_12$ (94)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x{-}y),\frac{1}{2}(x{+}y),z;\ +(\frac{1}{2},\frac{1}{2},0)$	$2a;2b$	$4d$	$4f$	$4e$	$4c$	$4d$	$2\times4c$ $2\times4f$	$2\times4d$ $8g$	$8g$ $8g$	$2\times4e$ $8g$	$8g$ $2\times8g$
[2] $P4_22_12$ (94)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x{-}y){+}\frac{1}{2},\frac{1}{2}(x{+}y),z;\ +(\frac{1}{2},\frac{1}{2},0)$	$4d$	$2a;2b$	$4e$	$4f$	$4d$	$4c$	$2\times4d$ $8g$	$2\times4c$ $2\times4e$	$8g$ $8g$	$8g$ $8g$	$2\times4f$ $2\times8g$
[2] $P4_122$ (91)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$4a$	$4b$	$4a$	$4b$	$4c$	$4c$	$8d$ $2\times4a$	$8d$ $8d$	$8d$ $8d$	$8d$ $2\times4c$	$2\times4b$ $2\times8d$
[2] $P4_122$ (91)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z{+}\frac{1}{4};\ +(0,0,\frac{1}{2})$	$4a$	$4b$	$4b$	$4a$	$4c$	$4c$	$8d$ $8d$	$8d$ $2\times4b$	$8d$ $2\times4c$	$2\times4a$ $8d$	$8d$ $2\times8d$
Enlarged unit cell, isomorphic													
[3] $P4_222$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4g$	$2b;4h$	$2c;4i$	$2d;4i$	$2e;4g$	$2f;4h$	$3\times4g$ $4l;8p$	$3\times4h$ $4m;8p$	$3\times4i$ $4o;8p$	$4j;8p$ $4n;8p$	$4k;8p$ $3\times8p$

Continued on preceding page

$P4_22_12$ No. 94 D_4^6

	Axes	Coordinates	Wyckoff positions 2*a*	2*b*	4*c*	4*d*	4*e*	4*f*	8*g*
I Maximal *translationengleiche* subgroups									
[2] $P4_2$ (77)		$x+\frac{1}{2},y,z$	$2c$	$2c$	$2\times2c$	$2a;2b$	$4d$	$4d$	$2\times4d$
[2] $P2_12_12$ (18)		$x,y,z+\frac{1}{4}$	$2a$	$2a$	$2\times2a$	$2\times2b$	$4c$	$4c$	$2\times4c$
[2] $C222$ (21)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$2a;2c$	$2b;2d$	$4i;4j$	$2\times4k$	$4f;4g$	$4e;4h$	$2\times8l$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $P4_32_12$ (96)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$4a$	$4a$	$8b$	$8b$	$2\times4a$	$8b$	$2\times8b$
[2] $P4_32_12$ (96)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4a$	$4a$	$8b$	$8b$	$8b$	$2\times4a$	$2\times8b$
[2] $P4_12_12$ (92)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$4a$	$4a$	$8b$	$8b$	$2\times4a$	$8b$	$2\times8b$
[2] $P4_12_12$ (92)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4a$	$4a$	$8b$	$8b$	$8b$	$2\times4a$	$2\times8b$
Enlarged unit cell, isomorphic									
[3] $P4_22_12$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4c$	$2b;4c$	$3\times4c$	$3\times4d$	$4e;8g$	$4f;8g$	$3\times8g$
[p] $P4_22_12$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=\text{prime}>2$;	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4c$	$2b;\frac{p-1}{2}\times4c$	$p\times4c$	$p\times4d$	$4e;\frac{p-1}{2}\times8g$	$4f;\frac{p-1}{2}\times8g$	$p\times8g$
[9] $P4_22_12$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4e;4f;8g$	$2b;4e;4f;8g$	$4c;4\times8g$	$4d;4\times8g$	$3\times4e;3\times8g$	$3\times4f;3\times8g$	$9\times8g$
[p^2] $P4_22_12$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=\text{prime}>2$;	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4e$; $\frac{p-1}{2}\times4f$; $\frac{(p-1)^2}{4}\times8g$	$2b;\frac{p-1}{2}\times4e$; $\frac{p-1}{2}\times4f$; $\frac{(p-1)^2}{4}\times8g$	$4c$; $\frac{p^2-1}{2}\times8g$	$4d$; $\frac{p^2-1}{2}\times8g$	$p\times4e$; $\frac{p(p-1)}{2}\times8g$	$p\times4f$; $\frac{p(p-1)}{2}\times8g$	$p^2\times8g$

D_4^7 No. 95 $P4_322$

	Axes	Coordinates	Wyckoff positions 4a	4b	4c	8d
I Maximal *translationengleiche* subgroups						
[2] $P4_3$ (78)			$4a$	$4a$	$4a$	$2\times4a$
[2] $P222_1$ (17)		$x,y,z+\frac{1}{4}$	$2a;2c$	$2b;2d$	$4e$	$2\times4e$
[2] $C222_1$ (20)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y),\frac{1}{2}(-x+y),z-\frac{1}{8}$	$8c$	$8c$	$4a;4b$	$2\times8c$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $P4_32_12$ (96)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y),\frac{1}{2}(-x+y),z; +(\frac{1}{2},\frac{1}{2},0)$	$2\times4a$	$8b$	$8b$	$2\times8b$
[2] $P4_32_12$ (96)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{2},\frac{1}{2}(-x+y),z; +(\frac{1}{2},\frac{1}{2},0)$	$8b$	$2\times4a$	$8b$	$2\times8b$
Enlarged unit cell, isomorphic						
[3] $P4_122$ (91)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$4a;8d$	$4b;8d$	$4c;8d$	$3\times8d$
[p] $P4_122$ (91)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime $=4n-1$; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z; +(0,0,\frac{u}{p})$	$4a; \frac{p-1}{2}\times8d$	$4b; \frac{p-1}{2}\times8d$	$4c; \frac{p-1}{2}\times8d$	$p\times8d$
[5] $P4_322$	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x,y,\frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$	$4a;2\times8d$	$4b;2\times8d$	$4c;2\times8d$	$5\times8d$
[p] $P4_322$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime $=4n+1$; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z; +(0,0,\frac{u}{p})$	$4a; \frac{p-1}{2}\times8d$	$4b; \frac{p-1}{2}\times8d$	$4c; \frac{p-1}{2}\times8d$	$p\times8d$
[2] $P4_322$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y),\frac{1}{2}(-x+y),z+\frac{1}{8}; +(\frac{1}{2},\frac{1}{2},0)$	$2\times4c$	$8d$	$4a;4b$	$2\times8d$
[2] $P4_322$	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)+\frac{1}{2},\frac{1}{2}(-x+y),z+\frac{1}{8}; +(\frac{1}{2},\frac{1}{2},0)$	$8d$	$2\times4c$	$4a;4b$	$2\times8d$
[9] $P4_322$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$3\times4a;3\times8d$	$3\times4b;3\times8d$	$3\times4c;3\times8d$	$9\times8d$
[p^2] $P4_322$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime >2; $u,v=1,\ldots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z; +(\frac{u}{p},\frac{v}{p},0)$	$p\times4a;$ $\frac{p(p-1)}{2}\times8d$	$p\times4b;$ $\frac{p(p-1)}{2}\times8d$	$p\times4c;$ $\frac{p(p-1)}{2}\times8d$	$p^2\times8d$

$P4_32_12$ No. 96 D_4^8

	Axes	Coordinates	Wyckoff positions	
			$4a$	$8b$
I Maximal *translationengleiche* subgroups				
[2] $P4_3$ (78)		$x+\frac{1}{2}, y, z$	$4a$	$2\times 4a$
[2] $P2_12_12_1$ (19)		$x+\frac{1}{4}, y, z-\frac{1}{8}$	$4a$	$2\times 4a$
[2] $C222_1$ (20)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z$	$4a; 4b$	$2\times 8c$
II Maximal *klassengleiche* subgroups				
Enlarged unit cell, isomorphic				
[3] $P4_12_12$ (92)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$4a; 8b$	$3\times 8b$
[p] $P4_12_12$ (92)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$4a; \frac{p-1}{2}\times 8b$	$p\times 8b$
	p = prime $= 4n-1$; $u = 1,\ldots,p-1$			
[5] $P4_32_12$	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$	$4a; 2\times 8b$	$5\times 8b$
[p] $P4_32_12$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$4a; \frac{p-1}{2}\times 8b$	$p\times 8b$
	p = prime $= 4n+1$; $u = 1,\ldots,p-1$			
[9] $P4_32_12$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$3\times 4a; 3\times 8b$	$9\times 8b$
[p^2] $P4_32_12$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$p\times 4a; \frac{p(p-1)}{2}\times 8b$	$p^2\times 8b$
	p = prime > 2; $u, v = 1,\ldots,p-1$			

D_4^9 No. 97 $I422$

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$4c$	$4d$	$4e$	$8f$
				$8g$	$8h$	$8i$	$8j$	$16k$
I Maximal *translationengleiche* subgroups								
[2] $I4$			$2a$	$2a$	$4b$	$4b$	$2\times2a$	$2\times4b$
(79)				$8c$	$8c$	$8c$	$8c$	$2\times8c$
[2] $I222$			$2a$	$2c$	$2b;2d$	$4j$	$4i$	$2\times4j$
(23)				$8k$	$4e;4g$	$4f;4h$	$8k$	$2\times8k$
[2] $F222$	$\mathbf{a}-\mathbf{b}$,	$\frac{1}{2}(x-y)$,	$4a$	$4b$	$8h$	$4c;4d$	$8g$	$2\times8h$
(22)	$\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x+y),z$		$8e;8f$	$16k$	$16k$	$8i;8j$	$2\times16k$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P4_22_12$			$2a$	$2b$	$4d$	$4d$	$4c$	$2\times4d$
(94)				$4e;4f$	$8g$	$8g$	$8g$	$2\times8g$
[2] $P4_222$		$x+\frac{1}{2},y,z$	$2d$	$2c$	$2a;2b$	$2e;2f$	$4i$	$4g;4h$
(93)				$8p$	$4j;4k$	$4l;4m$	$4n;4o$	$2\times8p$
[2] $P42_12$		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2c$	$2c$	$4d$	$2a;2b$	$2\times2c$	$2\times4d$
(90)				$8g$	$8g$	$8g$	$4e;4f$	$2\times8g$
[2] $P422$			$1a;1d$	$1b;1c$	$2e;2f$	$4i$	$2g;2h$	$2\times4i$
(89)				$4j;4k$	$4l;4m$	$4n;4o$	$8p$	$2\times8p$
Enlarged unit cell, isomorphic								
[3] $I422$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$4c;8f$	$4d;8f$	$3\times4e$	$3\times8f$
				$8g;16k$	$8h;16k$	$8i;16k$	$8j;16k$	$3\times16k$
[p] $I422$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$4c;\frac{p-1}{2}\times8f$	$4d;\frac{p-1}{2}\times8f$	$p\times4e$	$p\times8f$
$p=$ prime >2;		$u=1,\ldots,p-1$		$8g;\frac{p-1}{2}\times16k$	$8h;\frac{p-1}{2}\times16k$	$8i;\frac{p-1}{2}\times16k$	$8j;\frac{p-1}{2}\times16k$	$p\times16k$
[9] $I422$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;8g;8h$	$2b;8g;8i$	$4c;8h;8i;16k$	$4d;2\times8j;16k$	$4e;2\times16k$	$8f;4\times16k$
				$3\times8g;3\times16k$	$3\times8h;3\times16k$	$3\times8i;3\times16k$	$3\times8j;3\times16k$	$9\times16k$
[p^2] $I422$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;$ $+(\frac{u}{p},\frac{v}{p},0)$	$2a;\frac{p-1}{2}\times8g;$ $\frac{p-1}{2}\times8h;$ $\frac{(p-1)(p-3)}{8}\times16k$	$2b;\frac{p-1}{2}\times8g;$ $\frac{p-1}{2}\times8i;$ $\frac{(p-1)(p-3)}{8}\times16k$	$4c;\frac{p-1}{2}\times8h;$ $\frac{p-1}{2}\times8i;$ $\frac{(p-1)^2}{4}\times16k$	$4d;(p-1)\times8j;$ $\frac{(p-1)^2}{4}\times16k$	$4e;\frac{p^2-1}{4}\times16k$	$8f;\frac{p^2-1}{2}\times16k$
$p=$ prime >2;		$u,v=1,\ldots,p-1$		$p\times8g;$ $\frac{p(p-1)}{2}\times16k$	$p\times8h;$ $\frac{p(p-1)}{2}\times16k$	$p\times8i;$ $\frac{p(p-1)}{2}\times16k$	$p\times8j;$ $\frac{p(p-1)}{2}\times16k$	$p^2\times16k$

$I4_122$ No. 98 D_4^{10}

	Axes	Coordinates	Wyckoff positions 4a	4b	8c	8d	8e	8f	16g
I Maximal *translationengleiche* subgroups									
[2] $I4_1$ (80)			$4a$	$4a$	$2\times4a$	$8b$	$8b$	$8b$	$2\times8b$
[2] $I2_12_12_1$ (24)		$x,y+\frac{1}{4},z+\frac{1}{8}$	$4c$	$4c$	$2\times4c$	$8d$	$8d$	$4a;4b$	$2\times8d$
[2] $F222$ (22)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$4a;4d$	$4b;4c$	$8g;8h$	$8f;8j$	$8e;8i$	$16k$	$2\times16k$
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $P4_32_12$ (96)		$x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	$4a$	$4a$	$8b$	$8b$	$2\times4a$	$8b$	$2\times8b$
[2] $P4_322$ (95)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{8}$	$4c$	$4c$	$8d$	$2\times4c$	$8d$	$4a;4b$	$2\times8d$
[2] $P4_12_12$ (92)		$x+\frac{1}{4},y+\frac{1}{4},z$	$4a$	$4a$	$8b$	$2\times4a$	$8b$	$8b$	$2\times8b$
[2] $P4_122$ (91)		$x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{8}$	$4c$	$4c$	$8d$	$8d$	$2\times4c$	$4a;4b$	$2\times8d$
Enlarged unit cell, isomorphic									
[3] $I4_122$	$\mathbf{b},-\mathbf{a},3\mathbf{c}$	$y,-x,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$4a;8c$	$4b;8c$	$3\times8c$	$8e;16g$	$8d;16g$	$8f;16g$	$3\times16g$
[p] $I4_122$	$\mathbf{b},-\mathbf{a},p\mathbf{c}$; $p=\text{prime}=4n-1$;	$y,-x,\frac{1}{p}z;+(0,0,\frac{u}{p})$; $u=1,\ldots,p-1$	$4a;\frac{p-1}{2}\times8c$	$4b;\frac{p-1}{2}\times8c$	$p\times8c$	$8e;\frac{p-1}{2}\times16g$	$8d;\frac{p-1}{2}\times16g$	$8f;\frac{p-1}{2}\times16g$	$p\times16g$
[5] $I4_122$	$\mathbf{a},\mathbf{b},5\mathbf{c}$	$x,y,\frac{1}{5}z;\pm(0,0,\frac{1}{5})$; $\pm(0,0,\frac{2}{5})$	$4a;2\times8c$	$4b;2\times8c$	$5\times8c$	$8d;2\times16g$	$8e;2\times16g$	$8f;2\times16g$	$5\times16g$
[p] $I4_122$	$\mathbf{a},\mathbf{b},p\mathbf{c}$; $p=\text{prime}=4n+1$;	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$; $u=1,\ldots,p-1$	$4a;\frac{p-1}{2}\times8c$	$4b;\frac{p-1}{2}\times8c$	$p\times8c$	$8d;\frac{p-1}{2}\times16g$	$8e;\frac{p-1}{2}\times16g$	$8f;\frac{p-1}{2}\times16g$	$p\times16g$
[9] $I4_122$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z$; $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$4a;8d;8e;16g$	$4b;8d;8e;16g$	$8c;4\times16g$	$3\times8d;3\times16g$	$3\times8e;3\times16g$	$3\times8f;3\times16g$	$9\times16g$
[p^2] $I4_122$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$; $p=\text{prime}>2$;	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$; $u,v=1,\ldots,p-1$	$4a;\frac{p-1}{2}\times8d$; $\frac{p-1}{2}\times8e$; $\frac{(p-1)^2}{4}\times16g$	$4b;\frac{p-1}{2}\times8d$; $\frac{p-1}{2}\times8e$; $\frac{(p-1)^2}{4}\times16g$	$8c$; $\frac{p^2-1}{2}\times16g$	$p\times8d$; $\frac{p(p-1)}{2}\times16g$	$p\times8e$; $\frac{p(p-1)}{2}\times16g$	$p\times8f$; $\frac{p(p-1)}{2}\times16g$	$p^2\times16g$

C_{4v}^{1} No. 99 *P4mm*

	Axes	Coordinates	$1a$	$1b$	$2c$	$4d$	$4e$	$4f$	$8g$
I Maximal *translationengleiche* subgroups									
[2] $P4$ (75)			$1a$	$1b$	$2c$	$4d$	$4d$	$4d$	$2\times4d$
[2] $Pmm2$ (25)			$1a$	$1d$	$1b;1c$	$4i$	$2e;2g$	$2f;2h$	$2\times4i$
[2] $Cmm2$ (35)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2a$	$2b$	$4c$	$4d;4e$	$8f$	$8f$	$2\times8f$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $I4cm$ (108)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a$	$4b$	$8c$	$16d$	$16d$	$2\times8c$	$2\times16d$
[2] $I4cm$ (108)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4b$	$4a$	$8c$	$16d$	$2\times8c$	$16d$	$2\times16d$
[2] $I4mm$ (107)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2\times2a$	$4b$	$8c$	$2\times8d$	$2\times8c$	$16e$	$2\times16e$
[2] $I4mm$ (107)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4b$	$2\times2a$	$8c$	$2\times8d$	$16e$	$2\times8c$	$2\times16e$
[2] $P4_2mc$ (105)	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a$	$2b$	$2\times2c$	$8f$	$2\times4d$	$2\times4e$	$2\times8f$
[2] $P4cc$ (103)	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a$	$2b$	$4c$	$8d$	$8d$	$8d$	$2\times8d$
[2] $P4_2cm$ (101)	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a$	$2b$	$4c$	$2\times4d$	$8e$	$8e$	$2\times8e$
[2] $P4bm$ (100)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$	$2b$	$4c$	$8d$	$8d$	$2\times4c$	$2\times8d$
[2] $P4bm$ (100)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2b$	$2a$	$4c$	$8d$	$2\times4c$	$8d$	$2\times8d$
Enlarged unit cell, isomorphic									
[2] $P4mm$	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2\times1a$	$2\times1b$	$2\times2c$	$2\times4d$	$2\times4e$	$2\times4f$	$2\times8g$
[3] $P4mm$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times1a$	$3\times1b$	$3\times2c$	$2\times4d$	$3\times4e$	$3\times4f$	$3\times8g$
[p] $P4mm$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime; $u = 1,\ldots,p-1$	$p\times1a$	$p\times1b$	$p\times2c$	$p\times4d$	$p\times4e$	$p\times4f$	$p\times8g$
[2] $P4mm$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a;1b$	$2c$	$4d$	$4e;4f$	$2\times4d$	$8g$	$2\times8g$
[2] $P4mm$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2c$	$1a;1b$	$4d$	$4e;4f$	$8g$	$2\times4d$	$2\times8g$
[9] $P4mm$	$3\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;4d;4e$	$1b;4d;4f$	$2c;4e;4f;8g$	$3\times4d$; $3\times8g$	$3\times4e$; $3\times8g$	$3\times4f$; $3\times8g$	$9\times8g$
[p^2] $P4mm$	$p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ p = prime > 2; $u, v = 1,\ldots,p-1$	$1a$; $\frac{p-1}{2}\times4d$; $\frac{p-1}{2}\times4e$; $\frac{(p-1)(p-3)}{8}\times8g$	$1b$; $\frac{p-1}{2}\times4d$; $\frac{p-1}{2}\times4f$; $\frac{(p-1)(p-3)}{8}\times8g$	$2c$; $\frac{p-1}{2}\times4e$; $\frac{p-1}{2}\times4f$; $\frac{(p-1)^2}{4}\times8g$	$p\times4d$; $\frac{p(p-1)}{2}\times8g$	$p\times4e$; $\frac{p(p-1)}{2}\times8g$	$p\times4f$; $\frac{p(p-1)}{2}\times8g$	$p^2\times8g$

$P4bm$ No. 100 C_{4v}^2

	Axes	Coordinates	Wyckoff positions 2*a*	2*b*	4*c*	8*d*
I Maximal *translationengleiche* subgroups						
[2] *P*4 (75)			1*a*; 1*b*	2*c*	4*d*	2×4*d*
[2] *Pba*2 (32)			2*a*	2*b*	4*c*	2×4*c*
[2] *Cmm*2 (35)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{4}, \frac{1}{2}(x+y)+\frac{1}{4}, z$	4*c*	2*a*; 2*b*	4*d*; 4*e*	2×8*f*
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $P4_2bc$ (106)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	4*a*	4*b*	8*c*	2×8*c*
[2] *P*4*nc* (104)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2×2*a*	4*b*	8*c*	2×8*c*
[2] $P4_2nm$ (102)	**a**, **b**, 2**c**	$x+\frac{1}{2}, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	4*b*	2×2*a*	2×4*c*	2×8*d*
Enlarged unit cell, isomorphic						
[2] *P*4*bm*	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2×2*a*	2×2*b*	2×4*c*	2×8*d*
[3] *P*4*bm*	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3×2*a*	3×2*b*	3×4*c*	3×8*d*
[*p*] *P*4*bm*	**a**, **b**, *p***c** p = prime; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	*p*×2*a*	*p*×2*b*	*p*×4*c*	*p*×8*d*
[9] *P*4*bm*	3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	2*a*; 2×8*d*	2*b*; 2×4*c*; 8*d*	3×4*c*; 3×8*d*	9×8*d*
[p^2] *P*4*bm*	*p***a**, *p***b**, **c** p = prime > 2; $u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	2*a*; $\frac{1}{4}(p^2-1)\times 8d$	2*b*; $(p-1)\times 4c$; $\frac{1}{4}(p-1)^2\times 8d$	$p\times 4c$; $\frac{1}{2}p(p-1)\times 8d$	$p^2\times 8d$

C_{4v}^{3} No. 101 $P4_2cm$

	Axes	Coordinates	Wyckoff positions				
			$2a$	$2b$	$4c$	$4d$	$8e$
I Maximal *translationengleiche* subgroups							
[2] $P4_2$ (77)			$2a$	$2b$	$2\times 2c$	$4d$	$2\times 4d$
[2] $Pcc2$ (27)			$2a$	$2d$	$2b; 2c$	$4e$	$2\times 4e$
[2] $Cmm2$ (35)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2\times 2a$	$2\times 2b$	$2\times 4c$	$4d; 4e$	$2\times 8f$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, non-isomorphic							
[2] $P4_2bc$ (106)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$4a$	$4b$	$8c$	$8c$	$2\times 8c$
[2] $P4_2bc$ (106)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$4b$	$4a$	$8c$	$8c$	$2\times 8c$
[2] $P4_2mc$ (105)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$2a; 2b$	$2\times 2c$	$8f$	$4d; 4e$	$2\times 8f$
[2] $P4_2mc$ (105)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z; +(\frac{1}{2}, \frac{1}{2}, 0)$	$2\times 2c$	$2a; 2b$	$8f$	$4d; 4e$	$2\times 8f$
Enlarged unit cell, isomorphic							
[3] $P4_2cm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3\times 2a$	$3\times 2b$	$3\times 4c$	$3\times 4d$	$3\times 8e$
[p] $P4_2cm$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$p\times 2a$	$p\times 2b$	$p\times 4c$	$p\times 4d$	$p\times 8e$
	p = prime > 2; $u = 1, \ldots, p-1$						
[9] $P4_2cm$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3}, 0, 0); \pm(0, \frac{1}{3}, 0); \pm(\frac{1}{3}, \frac{1}{3}, 0); \pm(\frac{1}{3}, \frac{2}{3}, 0)$	$2a; 2\times 4d; 8e$	$2b; 2\times 4d; 8e$	$4c; 4\times 8e$	$3\times 4d; 3\times 8e$	$9\times 8e$
[p^2] $P4_2cm$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime > 2; $u, v = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$	$2a; (p-1)\times 4d; \frac{1}{4}(p-1)^2\times 8e$	$2b; (p-1)\times 4d; \frac{1}{4}(p-1)^2\times 8e$	$4c; \frac{1}{2}(p^2-1)\times 8e$	$p\times 4d; \frac{1}{2}p(p-1)\times 8e$	$p^2\times 8e$

$P4_2nm$ No. 102 C_{4v}^4

	Axes	Coordinates	Wyckoff positions			
			$2a$	$4b$	$4c$	$8d$
I Maximal *translationengleiche* subgroups						
[2] $P4_2$ (77)		$x+\frac{1}{2},y,z$	$2c$	$2a;2b$	$4d$	$2\times4d$
[2] $Pnn2$ (34)			$2a$	$2\times2b$	$4c$	$2\times4c$
[2] $Cmm2$ (35)	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$2a;2b$	$2\times4c$	$4d;4e$	$2\times8f$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $I4_1cd$ (110)	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),\frac{1}{2}z;+(0,0,\frac{1}{2})$	$8a$	$16b$	$16b$	$2\times16b$
[2] $I4_1cd$ (110)	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),\frac{1}{2}z;+(0,0,\frac{1}{2})$	$8a$	$16b$	$16b$	$2\times16b$
[2] $I4_1md$ (109)	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2\times4a$	$16c$	$2\times8b$	$2\times16c$
[2] $I4_1md$ (109)	$\mathbf{a}-\mathbf{b},\mathbf{a}+\mathbf{b},2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2\times4a$	$16c$	$2\times8b$	$2\times16c$
Enlarged unit cell, isomorphic						
[3] $P4_2nm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times4b$	$3\times4c$	$3\times8d$
[p] $P4_2nm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ p = prime > 2; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$	$p\times2a$	$p\times4b$	$p\times4c$	$p\times8d$
[9] $P4_2nm$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times4c;8d$	$4b;4\times8d$	$3\times4c;3\times8d$	$9\times8d$
[p^2] $P4_2nm$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ p = prime > 2; $u,v=1,\dots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$	$2a;(p-1)\times4c;$ $\frac{1}{4}(p-1)^2\times8d$	$4b;$ $\frac{1}{2}(p^2-1)\times8d$	$p\times4c;$ $\frac{1}{2}p(p-1)\times8d$	$p^2\times8d$

C_{4v}^{5} No. 103 $P4cc$

	Axes	Coordinates	Wyckoff positions 2*a*	2*b*	4*c*	8*d*
I Maximal *translationengleiche* subgroups						
[2] $P4$ (75)			$2\times1a$	$2\times1b$	$2\times2c$	$2\times4d$
[2] $Pcc2$ (27)			$2a$	$2d$	$2b;2c$	$2\times4e$
[2] $Ccc2$ (37)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$4a$	$4b$	$2\times4c$	$2\times8d$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $P4nc$ (104)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$2\times2a$	$4b$	$8c$	$2\times8c$
[2] $P4nc$ (104)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$4b$	$2\times2a$	$8c$	$2\times8c$
Enlarged unit cell, isomorphic						
[3] $P4cc$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times4c$	$3\times8d$
[p] $P4cc$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime > 2; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times2a$	$p\times2b$	$p\times4c$	$p\times8d$
[2] $P4cc$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$2a;2b$	$4c$	$8d$	$2\times8d$
[2] $P4cc$	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$	$4c$	$2a;2b$	$8d$	$2\times8d$
[9] $P4cc$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times8d$	$2b;2\times8d$	$4c;4\times8d$	$9\times8d$
[p^2] $P4cc$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime > 2; $u,v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$2a; \frac{1}{4}(p^2-1)\times8d$	$2b; \frac{1}{4}(p^2-1)\times8d$	$4c; \frac{1}{2}(p^2-1)\times8d$	$p^2\times8d$

*P*4*nc* No. 104 C_{4v}^{6}

	Axes	Coordinates	2*a*	4*b*	8*c*
I Maximal *translationengleiche* subgroups					
[2] *P*4 (75)			1*a*; 1*b*	2×2*c*	2×4*d*
[2] *Pnn*2 (34)			2*a*	2×2*b*	2×4*c*
[2] *Ccc*2 (37)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{4}, \frac{1}{2}(x+y)+\frac{1}{4}, z$	4*c*	4*a*; 4*b*	2×8*d*
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, isomorphic					
[3] *P*4*nc*	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3×2*a*	3×4*b*	3×8*c*
[*p*] *P*4*nc*	**a**, **b**, *p***c** p = prime > 2; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	*p*×2*a*	*p*×4*b*	*p*×8*c*
[9] *P*4*nc*	3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	2*a*; 2×8*c*	4*b*; 4×8*c*	9×8*c*
[p^2] *P*4*nc*	*p***a**, *p***b**, **c** p = prime > 2; $u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	2*a*; $\frac{1}{4}(p^2-1)$×8*c*	4*b*; $\frac{1}{2}(p^2-1)$×8*c*	p^2×8*c*

C_{4v}^{7} No. 105 $P4_2mc$

	Axes	Coordinates	$2a$	$2b$	$2c$	$4d$	$4e$	$8f$
I Maximal *translationengleiche* subgroups								
[2] $P4_2$ (77)			$2a$	$2b$	$2c$	$4d$	$4d$	$2\times4d$
[2] $Pmm2$ (25)			$2\times1a$	$2\times1d$	$1b;1c$	$2e;2g$	$2f;2h$	$2\times4i$
[2] $Ccc2$ (37)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$4a$	$4b$	$4c$	$8d$	$8d$	$2\times8d$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P4_2nm$ (102)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2\times2a$	$4b$	$4c$	$2\times4c$	$8d$	$2\times8d$
[2] $P4_2nm$ (102)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4b$	$2\times2a$	$4c$	$8d$	$2\times4c$	$2\times8d$
[2] $P4_2cm$ (101)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2b$	$4c$	$4d$	$2\times4d$	$8e$	$2\times8e$
[2] $P4_2cm$ (101)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4c$	$2a;2b$	$4d$	$8e$	$2\times4d$	$2\times8e$
Enlarged unit cell, isomorphic								
[3] $P4_2mc$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times2c$	$3\times4d$	$3\times4e$	$3\times8f$
[p] $P4_2mc$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}>2;\ u=1,\ldots,p-1$	$p\times2a$	$p\times2b$	$p\times2c$	$p\times4d$	$p\times4e$	$p\times8f$
[9] $P4_2mc$	3**a**,3**b**,**c**	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times4d;8f$	$2b;2\times4e;8f$	$2c;4d;4e;8f$	$3\times4d;3\times8f$	$3\times4e;3\times8f$	$9\times8f$
[p^2] $P4_2mc$	p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>2;$ $u,v=1,\ldots,p-1$	$2a;(p-1)\times4d;$ $\frac{(p-1)^2}{4}\times8f$	$2b;(p-1)\times4e;$ $\frac{(p-1)^2}{4}\times8f$	$2c;\frac{p-1}{2}\times4d;$ $\frac{p-1}{2}\times4e;$ $\frac{(p-1)^2}{4}\times8f$	$p\times4d;$ $\frac{p(p-1)}{2}\times8f$	$p\times4e;$ $\frac{p(p-1)}{2}\times8f$	$p^2\times8f$

$P4_2bc$ No. 106 C_{4v}^8

	Axes	Coordinates	Wyckoff positions 4a	4b	8c
I Maximal *translationengleiche* subgroups					
[2] $P4_2$ (77)			$2a;2b$	$2\times 2c$	$2\times 4d$
[2] $Pba2$ (32)			$2\times 2a$	$2\times 2b$	$2\times 4c$
[2] $Ccc2$ (37)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}, \frac{1}{2}(x+y)+\frac{1}{4}, z$	$2\times 4c$	$4a;4b$	$2\times 8d$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, isomorphic					
[3] $P4_2bc$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times 4a$	$3\times 4b$	$3\times 8c$
[p] $P4_2bc$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times 4a$	$p\times 4b$	$p\times 8c$
	$p = \text{prime} > 2;\ u = 1,\ldots,p-1$				
[9] $P4_2bc$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$4a;4\times 8c$	$4b;4\times 8c$	$9\times 8c$
[p^2] $P4_2bc$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$4a;\frac{1}{2}(p^2-1)\times 8c$	$4b;\frac{1}{2}(p^2-1)\times 8c$	$p^2\times 8c$
	$p = \text{prime} > 2;\ u,v = 1,\ldots,p-1$				

C_{4v}^{9} No. 107 $I4mm$

	Axes	Coordinates	Wyckoff positions 2*a*	4*b*	8*c*	8*d*	16*e*
I Maximal *translationengleiche* subgroups							
[2] *I*4 (79)			2*a*	4*b*	8*c*	8*c*	2×8*c*
[2] *Imm*2 (44)			2*a*	2×2*b*	8*e*	4*c*; 4*d*	2×8*e*
[2] *Fmm*2 (42)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	4*a*	8*b*	8*c*; 8*d*	16*e*	2×16*e*
II Maximal *klassengleiche* subgroups							
Loss of centring translations							
[2] $P4_2mc$ (105)		$x+\frac{1}{2}, y, z$	2*c*	2*a*; 2*b*	8*f*	4*d*; 4*e*	2×8*f*
[2] *P*4*nc* (104)			2*a*	4*b*	8*c*	8*c*	2×8*c*
[2] $P4_2nm$ (102)			2*a*	4*b*	2×4*c*	8*d*	2×8*d*
[2] *P*4*mm* (99)			1*a*; 1*b*	2×2*c*	2×4*d*	4*e*; 4*f*	2×8*g*
Enlarged unit cell, isomorphic							
[3] *I*4*mm*	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	3×2*a*	3×4*b*	3×8*c*	3×8*d*	3×16*e*
[*p*] *I*4*mm*	**a**, **b**, *p***c**	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	*p*×2*a*	*p*×4*b*	*p*×8*c*	*p*×8*d*	*p*×16*e*
	p = prime > 2; $u = 1, \ldots, p-1$						
[9] *I*4*mm*	3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3}, 0, 0)$; $\pm(0, \frac{1}{3}, 0)$; $\pm(\frac{1}{3}, \frac{1}{3}, 0)$; $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	2*a*; 8*c*; 8*d*	4*b*; 2×8*d*; 16*e*	3×8*c*; 3×16*e*	3×8*d*; 3×16*e*	9×16*e*
[p^2] *I*4*mm*	*p***a**, *p***b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$	$2a$; $\frac{p-1}{2}\times 8c$; $\frac{p-1}{2}\times 8d$; $\frac{(p-1)(p-3)}{8}\times 16e$	$4b$; $(p-1)\times 8d$; $\frac{(p-1)^2}{4}\times 16e$	$p\times 8c$; $\frac{p(p-1)}{2}\times 16e$	$p\times 8d$; $\frac{p(p-1)}{2}\times 16e$	$p^2\times 16e$
	p = prime > 2; $u, v = 1, \ldots, p-1$						

$I4cm$ No. 108 C_{4v}^{10}

	Axes	Coordinates	Wyckoff positions			
			$4a$	$4b$	$8c$	$16d$
I Maximal *translationengleiche* subgroups						
[2] $I4$ (79)			$2\times 2a$	$4b$	$8c$	$2\times 8c$
[2] $Iba2$ (45)			$4a$	$4b$	$8c$	$2\times 8c$
[2] $Fmm2$ (42)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}, \frac{1}{2}(x+y)+\frac{1}{4}, z$	$8b$	$2\times 4a$	$8c; 8d$	$2\times 16e$
II Maximal *klassengleiche* subgroups						
Loss of centring translations						
[2] $P4_2bc$ (106)		$x+\frac{1}{2}, y, z$	$4b$	$4a$	$8c$	$2\times 8c$
[2] $P4cc$ (103)			$2a; 2b$	$4c$	$8d$	$2\times 8d$
[2] $P4_2cm$ (101)		$x+\frac{1}{2}, y, z$	$4c$	$2a; 2b$	$2\times 4d$	$2\times 8e$
[2] $P4bm$ (100)			$2\times 2a$	$2\times 2b$	$2\times 4c$	$2\times 8d$
Enlarged unit cell, isomorphic						
[3] $I4cm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times 4a$	$3\times 4b$	$3\times 8c$	$3\times 16d$
[p] $I4cm$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime > 2; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times 4a$	$p\times 4b$	$p\times 8c$	$p\times 16d$
[9] $I4cm$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$4a; 2\times 16d$	$4b; 2\times 8c; 16d$	$3\times 8c; 3\times 16d$	$9\times 16d$
[p^2] $I4cm$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime > 2; $u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$4a$; $\frac{1}{4}(p^2-1)\times 16d$	$4b; (p-1)\times 8c$; $\frac{1}{4}(p-1)^2\times 16d$	$p\times 8c$; $\frac{1}{2}p(p-1)\times 16d$	$p^2\times 16d$

C_{4v}^{11} No. 109 $I4_1md$

	Axes	Coordinates	Wyckoff positions 4*a*	8*b*	16*c*
I Maximal *translationengleiche* subgroups					
[2] $I4_1$ (80)			$4a$	$8b$	$2\times 8b$
[2] $Imm2$ (44)			$2a; 2b$	$4c; 4d$	$2\times 8e$
[2] $Fdd2$ (43)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z$	$8a$	$16b$	$2\times 16b$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, isomorphic					
[3] $I4_1md$	$\mathbf{b}, -\mathbf{a}, 3\mathbf{c}$	$y, -x, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times 4a$	$3\times 8b$	$3\times 16c$
[p] $I4_1md$	$\mathbf{b}, -\mathbf{a}, p\mathbf{c}$	$y, -x, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times 4a$	$p\times 8b$	$p\times 16c$
	$p = \text{prime} = 4n-1;\ u = 1,\dots,p-1$				
[5] $I4_1md$	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$	$5\times 4a$	$5\times 8b$	$5\times 16c$
[p] $I4_1md$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times 4a$	$p\times 8b$	$p\times 16c$
	$p = \text{prime} = 4n+1;\ u = 1,\dots,p-1$				
[9] $I4_1md$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0);$ $\pm(0,\frac{1}{3},0); \pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$4a; 2\times 8b; 16c$	$3\times 8b; 3\times 16c$	$9\times 16c$
[p^2] $I4_1md$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$4a; (p-1)\times 8b;$ $\frac{1}{4}(p-1)^2\times 16c$	$p\times 8b;$ $\frac{1}{2}p(p-1)\times 16c$	$p^2\times 16c$
	$p = \text{prime} > 2;\ u, v = 1,\dots,p-1$				

$I4_1cd$ No. 110 C_{4v}^{12}

	Axes	Coordinates	Wyckoff positions 8*a*	16*b*
I Maximal *translationengleiche* subgroups				
[2] $I4_1$ (80)			$2\times4a$	$2\times8b$
[2] $Iba2$ (45)			$4a;4b$	$2\times8c$
[2] $Fdd2$ (43)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$2\times8a$	$2\times16b$
II Maximal *klassengleiche* subgroups				
Enlarged unit cell, isomorphic				
[3] $I4_1cd$	**b**, −**a**, 3**c**	$y,-x,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times8a$	$3\times16b$
[p] $I4_1cd$	**b**, −**a**, p**c**	$y,-x,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}=4n-1;\ u=0,\dots,p-1$	$p\times8a$	$p\times16b$
[5] $I4_1cd$	**a**, **b**, 5**c**	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});\ \pm(0,0,\frac{2}{5})$	$5\times8a$	$5\times16b$
[p] $I4_1cd$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}=4n+1;\ u=0,\dots,p-1$	$p\times8a$	$p\times16b$
[9] $I4_1cd$	3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z;\ \pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$	$8a;4\times16b$	$9\times16b$
[p^2] $I4_1cd$	p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>2;\ u,v=1,\dots,p-1$	$8a;\frac{1}{2}(p^2-1)\times16b$	$p^2\times16b$

$P\bar{4}2m$ No. 111

CONTINUED (*from next page*)

	Axes	Coordinates	Wyckoff positions 1*a*	1*b* 2*g*	1*c* 2*h* 4*l*	1*d* 4*i* 4*m*	2*e* 4*j* 4*n*	2*f* 4*k* 8*o*
[p] $P\bar{4}2m$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}>2;$ $u=1,\dots,p-1$	$1a;\frac{p-1}{2}\times2g$	$1b;\frac{p-1}{2}\times2h$ $p\times2g$	$1c;\frac{p-1}{2}\times2g$ $p\times2h$ $4l;\frac{p-1}{2}\times8o$	$1d;\frac{p-1}{2}\times2h$ $4i;\frac{p-1}{2}\times8o$ $p\times4m$	$2e;\frac{p-1}{2}\times4m$ $4j;\frac{p-1}{2}\times8o$ $p\times4n$	$2f;\frac{p-1}{2}\times4m$ $4k;\frac{p-1}{2}\times8o$ $p\times8o$
[9] $P\bar{4}2m$	3**a**,3**b**,**c**	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;4i;4n$	$1b;4j;4n$ $2g;2\times4n;8o$	$1c;4k;4n$ $2h;2\times4n;8o$ $3\times4l;3\times8o$	$1d;4l;4n$ $3\times4i;3\times8o$ $4m;4\times8o$	$2e;4i;4l;8o$ $3\times4j;3\times8o$ $3\times4n;3\times8o$	$2f;4j;4k;8o$ $3\times4k;3\times8o$ $9\times8o$
[p^2] $P\bar{4}2m$	p**a**,p**b**,**c**	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>2;$ $u,v=1,\dots,p-1$	$1a;\frac{p-1}{2}\times4i;$ $\frac{p-1}{2}\times4n;$ $\frac{(p-1)(p-3)}{8}\times8o$	$1b;\frac{p-1}{2}\times4j;$ $\frac{p-1}{2}\times4n;$ $\frac{(p-1)(p-3)}{8}\times8o$ $2g;(p-1)\times4n;$ $\frac{(p-1)^2}{4}\times8o$	$1c;\frac{p-1}{2}\times4k;$ $\frac{p-1}{2}\times4n;$ $\frac{(p-1)(p-3)}{8}\times8o$ $2h;(p-1)\times4n;$ $\frac{(p-1)^2}{4}\times8o$ $p\times4l;$ $\frac{p(p-1)}{2}\times8o$	$1d;\frac{p-1}{2}\times4l;$ $\frac{p-1}{2}\times4n;$ $\frac{(p-1)(p-3)}{8}\times8o$ $p\times4i;$ $\frac{p(p-1)}{2}\times8o$ $4m;\frac{p^2-1}{2}\times8o$	$2e;\frac{p-1}{2}\times4i;$ $\frac{p-1}{2}\times4l;$ $\frac{(p-1)^2}{4}\times8o$ $p\times4j;$ $\frac{p(p-1)}{2}\times8o$ $p\times4n;$ $\frac{p(p-1)}{2}\times8o$	$2f;\frac{p-1}{2}\times4j;$ $\frac{p-1}{2}\times4k;$ $\frac{(p-1)^2}{4}\times8o$ $p\times4k;$ $\frac{p(p-1)}{2}\times8o$ $p^2\times8o$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 111, pp. 586–587.

D_{2d}^{1} No. 111 $P\bar{4}2m$

	Axes	Coordinates	Wyckoff positions											
			1*a*	1*b*	1*c*	1*d*	2*e*	2*f*	2*g*	2*h*	4*i*	4*j* 4*m*	4*k* 4*n*	4*l* 8*o*
I Maximal *translationengleiche* subgroups														
[2] $P\bar{4}$ (81)			1*a*	1*d*	1*b*	1*c*	2*g*	2*g*	2*e*	2*f*	4*h*	4*h* 2×2*g*	4*h* 4*h*	4*h* 2×4*h*
[2] *P*222 (16)			1*a*	1*h*	1*d*	1*e*	1*b*; 1*c*	1*f*; 1*g*	2*q*	2*t*	2*i*; 2*m*	2*l*; 2*p* 2*r*; 2*s*	2*j*; 2*n* 4*u*	2*k*; 2*o* 2×4*u*
[2] *Cmm*2 (35)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	2*a*	2*b*	2*a*	2*b*	4*c*	4*c*	2×2*a*	2×2*b*	8*f*	8*f* 2×4*c*	8*f* 4*d*; 4*e*	8*f* 2×8*f*
II Maximal *klassengleiche* subgroups														
Enlarged unit cell, non-isomorphic														
[2] $I\bar{4}c2$ (120)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	4*b*	4*c*	4*a*	4*d*	8*h*	8*e*	8*f*	8*g*	16*i*	16*i* 16*i*	2×8*e* 16*i*	2×8*h* 2×16*i*
[2] $I\bar{4}c2$ (120)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*a*	4*d*	4*b*	4*c*	8*e*	8*h*	8*f*	8*g*	2×8*e*	2×8*h* 16*i*	16*i* 16*i*	16*i* 2×16*i*
[2] $I\bar{4}m2$ (119)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*a*; 2*b*	2*c*; 2*d*	4*e*	4*f*	8*g*	8*h*	2×4*e*	2×4*f*	2×8*g*	2×8*h* 16*j*	16*j* 2×8*i*	16*j* 2×16*j*
[2] $I\bar{4}m2$ (119)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*e*	4*f*	2*a*; 2*b*	2*c*; 2*d*	8*h*	8*g*	2×4*e*	2×4*f*	16*j*	16*j* 16*j*	2×8*g* 2×8*i*	2×8*h* 2×16*j*
[2] $P\bar{4}b2$ (117)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	2*a*	2*d*	2*b*	2*c*	4*g*	4*h*	4*e*	4*f*	8*i*	2×4*h* 8*i*	8*i* 8*i*	2×4*g* 2×8*i*
[2] $P\bar{4}b2$ (117)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	2*c*	2*b*	2*d*	2*a*	4*g*	4*h*	4*f*	4*e*	2×4*g*	8*i* 8*i*	2×4*h* 8*i*	8*i* 2×8*i*
[2] $P\bar{4}m2$ (115)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	1*a*; 1*b*	2*g*	1*c*; 1*d*	2*g*	4*h*	4*i*	2*e*; 2*f*	2×2*g*	2×4*h*	8*l* 8*l*	2×4*i* 4*j*; 4*k*	8*l* 2×8*l*
[2] $P\bar{4}m2$ (115)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	2*g*	1*c*; 1*d*	2*g*	1*a*; 1*b*	4*h*	4*i*	2×2*g*	2*e*; 2*f*	8*l*	2×4*i* 8*l*	8*l* 4*j*; 4*k*	2×4*h* 2×8*l*
[2] $P\bar{4}2c$ (112)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*e*	2*c*	2*a*	2*f*	4*m*	2*b*; 2*d*	4*k*	4*l*	8*n*	4*h*; 4*i* 2×4*m*	4*g*; 4*j* 8*n*	8*n* 2×8*n*
[2] $P\bar{4}2c$ (112)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*a*	2*f*	2*e*	2*c*	2*b*; 2*d*	4*m*	4*k*	4*l*	4*g*; 4*j*	8*n* 2×4*m*	8*n* 8*n*	4*h*; 4*i* 2×8*n*
Enlarged unit cell, isomorphic														
[2] $P\bar{4}2m$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	1*a*; 1*c*	2*h*	2*g*	1*b*; 1*d*	2*e*; 2*f*	4*m*	2×2*g*	2×2*h*	4*i*; 4*k*	8*o* 2×4*m*	8*o* 2×4*n*	4*j*; 4*l* 2×8*o*
[2] $P\bar{4}2m$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*g*	1*b*; 1*d*	1*a*; 1*c*	2*h*	4*m*	2*e*; 2*f*	2×2*g*	2×2*h*	8*o*	4*j*; 4*l* 2×4*m*	4*i*; 4*k* 2×4*n*	8*o* 2×8*o*
[3] $P\bar{4}2m$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	1*a*; 2*g*	1*b*; 2*h*	1*c*; 2*g*	1*d*; 2*h*	2*e*; 4*m*	2*f*; 4*m*	3×2*g*	3×2*h*	4*i*; 8*o*	4*j*; 8*o* 3×4*m*	4*k*; 8*o* 3×4*n*	4*l*; 8*o* 3×8*o*

Continued on preceding page

$P\bar{4}2c$ No. 112 D_{2d}^2

	Axes	Coordinates	Wyckoff positions						
			$2a$ $4h$	$2b$ $4i$	$2c$ $4j$	$2d$ $4k$	$2e$ $4l$	$2f$ $4m$	$4g$ $8n$
I Maximal *translationengleiche* subgroups									
[2] $P\bar{4}$ (81)			$2e$ $4h$	$2g$ $4h$	$2f$ $4h$	$2g$ $2\times2e$	$1a;1b$ $2\times2f$	$1c;1d$ $2\times2g$	$4h$ $2\times4h$
[2] $P222$ (16)		$x,y,z+\frac{1}{4}$	$1a;1d$ $2k;2p$	$1c;1f$ $2l;2o$	$1e;1h$ $2i;2n$	$1b;1g$ $2\times2q$	$2q$ $2\times2t$	$2t$ $2r;2s$	$2j;2m$ $2\times4u$
[2] $Ccc2$ (37)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$4a$ $8d$	$4c$ $8d$	$4b$ $8d$	$4c$ $2\times4a$	$4a$ $2\times4b$	$4b$ $2\times4c$	$8d$ $2\times8d$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $P\bar{4}n2$ (118)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4e$ $2\times4f$	$4f$ $2\times4g$	$2c;2d$ $8i$	$4g$ $2\times4e$	$2a;2b$ $2\times4h$	$4h$ $8i$	$8i$ $2\times8i$
[2] $P\bar{4}n2$ (118)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},$ $\frac{1}{2}(x+y),z;+(\frac{1}{2},\frac{1}{2},0)$	$2c;2d$ $8i$	$4g$ $8i$	$4e$ $2\times4f$	$4f$ $2\times4h$	$4h$ $2\times4e$	$2a;2b$ $8i$	$2\times4g$ $2\times8i$
[2] $P\bar{4}c2$ (116)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2b$ $8j$	$4e$ $8j$	$4i$ $2\times4f$	$4f$ $4g;4h$	$2c;2d$ $2\times4i$	$4i$ $8j$	$2\times4e$ $2\times8j$
[2] $P\bar{4}c2$ (116)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},$ $\frac{1}{2}(x+y),z;+(\frac{1}{2},\frac{1}{2},0)$	$4i$ $2\times4f$	$4f$ $2\times4e$	$2a;2b$ $8j$	$4e$ $2\times4i$	$4i$ $4g;4h$	$2c;2d$ $8j$	$8j$ $2\times8j$
Enlarged unit cell, isomorphic									
[3] $P\bar{4}2c$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4k$ $4i;8n$	$2d;4m$ $4h;8n$	$2c;4l$ $4g;8n$	$2b;4m$ $3\times4k$	$2e;4k$ $3\times4l$	$2f;4l$ $3\times4m$	$4j;8n$ $3\times8n$
[p] $P\bar{4}2c$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $p=\text{prime}>2;u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4k$ $4h(i^*);$ $\frac{p-1}{2}\times8n$	$2b(d^*);$ $\frac{p-1}{2}\times4m$ $4i(h^*);$ $\frac{p-1}{2}\times8n$	$2c;\frac{p-1}{2}\times4l$ $4j(g^*);$ $\frac{p-1}{2}\times8n$	$2d(b^*);$ $\frac{p-1}{2}\times4m$ $p\times4k$	$2e;$ $\frac{p-1}{2}\times4k$ $p\times4l$	$2f;$ $\frac{p-1}{2}\times4l$ $p\times4m$	$4g(j^*);$ $\frac{p-1}{2}\times8n$ $p\times8n$
[9] $P\bar{4}2c$	$3\mathbf{a}$, $3\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4g;4j;8n$ $3\times4h;3\times8n$	$2b;4g;4h;8n$ $3\times4i;3\times8n$	$2c;4h;4i;8n$ $3\times4j;3\times8n$	$2d;4i;4j;8n$ $4k;4\times8n$	$2e;2\times8n$ $4l;4\times8n$	$2f;2\times8n$ $4m;4\times8n$	$3\times4g;3\times8n$ $9\times8n$
[p^2] $P\bar{4}2c$	$p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>2;$ $u,v=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4g;$ $\frac{p-1}{2}\times4j;$ $\frac{(p-1)^2}{4}\times8n$ $p\times4h;$ $\frac{p(p-1)}{2}\times8n$	$2b;\frac{p-1}{2}\times4g;$ $\frac{p-1}{2}\times4h;$ $\frac{(p-1)^2}{4}\times8n$ $p\times4i;$ $\frac{p(p-1)}{2}\times8n$	$2c;\frac{p-1}{2}\times4h;$ $\frac{p-1}{2}\times4i;$ $\frac{(p-1)^2}{4}\times8n$ $p\times4j;$ $\frac{p(p-1)}{2}\times8n$	$2d;\frac{p-1}{2}\times4i;$ $\frac{p-1}{2}\times4j;$ $\frac{(p-1)^2}{4}\times8n$ $4k;\frac{p^2-1}{2}\times8n$	$2e;$ $\frac{p^2-1}{4}\times8n$ $4l;$ $\frac{p^2-1}{2}\times8n$	$2f;$ $\frac{p^2-1}{4}\times8n$ $4m;$ $\frac{p^2-1}{2}\times8n$	$p\times4g;$ $\frac{p(p-1)}{2}\times8n$ $p^2\times8n$

$^*p=4n-1$

D^3_{2d} No. 113 $P\bar{4}2_1m$

	Axes	Coordinates	Wyckoff positions 2*a*	2*b*	2*c*	4*d*	4*e*	8*f*
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}$ (81)			$1a; 1c$	$1b; 1d$	$2g$	$2e; 2f$	$4h$	$2\times4h$
[2] $P2_12_12$ (18)			$2a$	$2a$	$2b$	$2\times2a$	$4c$	$2\times4c$
[2] $Cmm2$ (35)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{4}, \frac{1}{2}(x+y)+\frac{1}{4}, z$	$4c$	$4c$	$2a; 2b$	$2\times4c$	$4d; 4e$	$2\times8f$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P\bar{4}2_1c$ (114)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a; 2b$	$4c$	$4d$	$2\times4c$	$8e$	$2\times8e$
[2] $P\bar{4}2_1c$ (114)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4c$	$2a; 2b$	$4d$	$2\times4c$	$8e$	$2\times8e$
Enlarged unit cell, isomorphic								
[2] $P\bar{4}2_1m$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a; 2b$	$4d$	$2\times2c$	$2\times4d$	$2\times4e$	$2\times8f$
[2] $P\bar{4}2_1m$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4d$	$2a; 2b$	$2\times2c$	$2\times4d$	$2\times4e$	$2\times8f$
[3] $P\bar{4}2_1m$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$2a; 4d$	$2b; 4d$	$3\times2c$	$3\times4d$	$3\times4e$	$3\times8f$
[p] $P\bar{4}2_1m$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$ p = prime > 2; $u = 1,\ldots,p-1$	$2a; \frac{p-1}{2}\times4d$	$2b; \frac{p-1}{2}\times4d$	$p\times2c$	$p\times4d$	$p\times4e$	$p\times8f$
[9] $P\bar{4}2_1m$	3**a**,3**b**,**c**	$\frac{1}{3}x, \frac{1}{3}y, z;$ $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$2a; 2\times8f$	$2b; 2\times8f$	$2c; 2\times4e; 8f$	$4d; 4\times8f$	$3\times4e; 3\times8f$	$9\times8f$
[p^2] $P\bar{4}2_1m$	p**a**,p**b**,**c**	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$ p = prime > 2; $u, v = 1,\ldots,p-1$	$2a; \frac{p^2-1}{4}\times8f$	$2b; \frac{p^2-1}{4}\times8f$	$2c; (p-1)\times4e;$ $\frac{(p-1)^2}{4}\times8f$	$4d; \frac{p^2-1}{2}\times8f$	$p\times4e;$ $\frac{p(p-1)}{2}\times8f$	$p^2\times8f$

$P\bar{4}2_1c$ No. 114 D_{2d}^4

Axes	Coordinates	Wyckoff positions				
		$2a$	$2b$	$4c$	$4d$	$8e$
I Maximal *translationengleiche* subgroups						
[2] $P\bar{4}$ (81)		$1a;1d$	$1b;1c$	$2e;2f$	$2\times 2g$	$2\times 4h$
[2] $P2_12_12$ (18)	$x,y,z+\frac{1}{4}$	$2a$	$2a$	$2\times 2a$	$2\times 2b$	$2\times 4c$
[2] $Ccc2$ (37) **a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{4},\frac{1}{2}(x+y)+\frac{1}{4},z$	$4c$	$4c$	$2\times 4c$	$4a;4b$	$2\times 8d$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[3] $P\bar{4}2_1c$ **a**, **b**, 3**c**	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4c$	$2b;4c$	$3\times 4c$	$3\times 4d$	$3\times 8e$
[p] $P\bar{4}2_1c$ **a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$; p = prime > 2; $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times 4c$	$2b;\frac{p-1}{2}\times 4c$	$p\times 4c$	$p\times 4d$	$p\times 8e$
[9] $P\bar{4}2_1c$ 3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z;\ \pm(\frac{1}{3},0,0);\ \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\ \pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times 8e$	$2b;2\times 8e$	$4c;4\times 8e$	$4d;4\times 8e$	$9\times 8e$
[p^2] $P\bar{4}2_1c$ p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$; p = prime > 2; $u,v=1,\ldots,p-1$	$2a;\frac{p^2-1}{4}\times 8e$	$2b;\frac{p^2-1}{4}\times 8e$	$4c;\frac{p^2-1}{2}\times 8e$	$4d;\frac{p^2-1}{2}\times 8e$	$p^2\times 8e$

$P\bar{4}m2$ No. 115

CONTINUED (*from next page*)

Axes	Coordinates	Wyckoff positions					
		$1a$ / $2g$	$1b$ / $4h$	$1c$ / $4i$	$1d$ / $4j$	$2e$ / $4k$	$2f$ / $8l$
[9] $P\bar{4}m2$ 3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;4h;4j$	$1b;4h;4k$	$1c;4i;4k$	$1d;4i;4j$	$2e;2\times 4j;8l$	$2f;2\times 4k;8l$
		$2g;4j;4k;8l$	$3\times 4h;3\times 8l$	$3\times 4i;3\times 8l$	$3\times 4j;3\times 8l$	$3\times 4k;3\times 8l$	$9\times 8l$
[p^2] $P\bar{4}m2$ p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$; p = prime > 2; $u,v=1,\ldots,p-1$	$1a;\frac{p-1}{2}\times 4h;$ $\frac{p-1}{2}\times 4j;$ $\frac{(p-1)(p-3)}{8}\times 8l$	$1b;\frac{p-1}{2}\times 4h;$ $\frac{p-1}{2}\times 4k;$ $\frac{(p-1)(p-3)}{8}\times 8l$	$1c;\frac{p-1}{2}\times 4i;$ $\frac{p-1}{2}\times 4k;$ $\frac{(p-1)(p-3)}{8}\times 8l$	$1d;\frac{p-1}{2}\times 4i;$ $\frac{p-1}{2}\times 4j;$ $\frac{(p-1)(p-3)}{8}\times 8l$	$2e;(p-1)\times 4j;$ $\frac{(p-1)^2}{4}\times 8l$	$2f;(p-1)\times 4k;$ $\frac{(p-1)^2}{4}\times 8l$
		$2g;\frac{p-1}{2}\times 4j;$ $\frac{p-1}{2}\times 4k;$ $\frac{(p-1)^2}{4}\times 8l$	$p\times 4h;$ $\frac{p(p-1)}{2}\times 8l$	$p\times 4i;$ $\frac{p(p-1)}{2}\times 8l$	$p\times 4j;$ $\frac{p(p-1)}{2}\times 8l$	$p\times 4k;\frac{p(p-1)}{2}\times 8l$	$p^2\times 8l$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 115, pp. 590–591.

D_{2d}^5 No. 115 $P\bar{4}m2$

	Axes	Coordinates	Wyckoff positions						
			$1a$	$1b$	$1c$	$1d$	$2e$ $4i$	$2f$ $4j$	$2g$ $4k$	$4h$ $8l$
I Maximal *translationengleiche* subgroups										
[2] $P\bar{4}$ (81)			$1a$	$1c$	$1d$	$1b$	$2e$ $4h$	$2f$ $4h$	$2g$ $4h$	$4h$ $2\times4h$
[2] $Pmm2$ (25)			$1a$	$1d$	$1d$	$1a$	$2\times1a$ $4i$	$2\times1d$ $2e;2g$	$1b;1c$ $2f;2h$	$4i$ $2\times4i$
[2] $C222$ (21)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$2a$	$2b$	$2c$	$2d$	$4i$ $4f;4h$	$4j$ $8l$	$4k$ $8l$	$4e;4g$ $2\times8l$
II Maximal *klassengleiche* subgroups										
Enlarged unit cell, non-isomorphic										
[2] $I\bar{4}2m$ (121)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),\frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$2a;2b$	$4c$	$4d$	$4e$	$2\times4e$ $16j$	$8h$ $2\times8i$	$8i$ $16j$	$8f;8g$ $2\times16j$
[2] $I\bar{4}2m$ (121)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),$ $\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4e$	$4d$	$4c$	$2a;2b$	$2\times4e$ $8f;8g$	$8h$ $2\times8i$	$8i$ $16j$	$16j$ $2\times16j$
[2] $I\bar{4}2m$ (121)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),\frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	$4c$	$2a;2b$	$4e$	$4d$	$8h$ $16j$	$2\times4e$ $16j$	$8i$ $2\times8i$	$8f;8g$ $2\times16j$
[2] $I\bar{4}2m$ (121)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),$ $\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$4d$	$4e$	$2a;2b$	$4c$	$8h$ $8f;8g$	$2\times4e$ $16j$	$8i$ $2\times8i$	$16j$ $2\times16j$
[2] $P\bar{4}c2$ (116)	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2c$	$2d$	$2b$	$2a$	$4g$ $4e;4f$	$4h$ $8j$	$4i$ $8j$	$8j$ $2\times8j$
[2] $P\bar{4}c2$ (116)	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$2a$	$2b$	$2d$	$2c$	$4g$ $8j$	$4h$ $8j$	$4i$ $8j$	$4e;4f$ $2\times8j$
[2] $P\bar{4}2_1m$ (113)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a$	$2c$	$2c$	$2b$	$4d$ $8f$	$2\times2c$ $8f$	$4e$ $2\times4e$	$8f$ $2\times8f$
[2] $P\bar{4}2_1m$ (113)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2c$	$2a$	$2b$	$2c$	$2\times2c$ $8f$	$4d$ $2\times4e$	$4e$ $8f$	$8f$ $2\times8f$
[2] $P\bar{4}2m$ (111)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$1a;1d$	$2e$	$2f$	$1b;1c$	$2g;2h$ $4j;4k$	$4m$ $2\times4n$	$4n$ $8o$	$4i;4l$ $2\times8o$
[2] $P\bar{4}2m$ (111)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2e$	$1a;1d$	$1b;1c$	$2f$	$4m$ $4j;4k$	$2g;2h$ $8o$	$4n$ $2\times4n$	$4i;4l$ $2\times8o$
Enlarged unit cell, isomorphic										
[2] $P\bar{4}m2$	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$1a;1d$	$1b;1c$	$2f$	$2e$	$2\times2e$ $8l$	$2\times2f$ $2\times4j$	$2\times2g$ $2\times4k$	$4h;4i$ $2\times8l$
[2] $P\bar{4}m2$	$\mathbf{a}$, $\mathbf{b}$, $2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$2e$	$2f$	$1b;1c$	$1a;1d$	$2\times2e$ $4h;4i$	$2\times2f$ $2\times4j$	$2\times2g$ $2\times4k$	$8l$ $2\times8l$
[3] $P\bar{4}m2$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$1a;2e$	$1b;2f$	$1c;2f$	$1d;2e$	$3\times2e$ $4i;8l$	$3\times2f$ $3\times4j$	$3\times2g$ $3\times4k$	$4h;8l$ $3\times8l$
[p] $P\bar{4}m2$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\ldots,p-1$	$1a;\frac{p-1}{2}\times2e$	$1b;\frac{p-1}{2}\times2f$	$1c;\frac{p-1}{2}\times2f$	$1d;\frac{p-1}{2}\times2e$	$p\times2e$ $4i;\frac{p-1}{2}\times8l$	$p\times2f$ $p\times4j$	$p\times2g$ $p\times4k$	$4h;\frac{p-1}{2}\times8l$ $p\times8l$

Continued on preceding page

$P\bar{4}c2$ No. 116 D_{2d}^{6}

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$2c$ $4g$	$2d$ $4h$	$4e$ $4i$	$4f$ $8j$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}$ (81)			$2e$	$2f$	$1a;1b$ $2\times2e$	$1c;1d$ $2\times2f$	$4h$ $2\times2g$	$4h$ $2\times4h$
[2] $Pcc2$ (27)			$2a$	$2d$	$2a$ $2\times2a$	$2d$ $2\times2d$	$4e$ $2b;2c$	$4e$ $2\times4e$
[2] $C222$ (21)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z+\frac{1}{4}$	$2a;2d$	$2b;2c$	$4i$ $2\times4i$	$4j$ $2\times4j$	$4e;4h$ $2\times4k$	$4f;4g$ $2\times8l$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P\bar{4}2_1c$ (114)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4c$	$4d$	$2a;2b$ $2\times4c$	$4d$ $2\times4d$	$8e$ $8e$	$8e$ $2\times8e$
[2] $P\bar{4}2_1c$ (114)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4d$	$4c$	$4d$ $2\times4d$	$2a;2b$ $2\times4c$	$8e$ $8e$	$8e$ $2\times8e$
[2] $P\bar{4}2c$ (112)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2c$	$2b;2d$	$2e;2f$ $4k;4l$	$4m$ $2\times4m$	$4h;4j$ $8n$	$4g;4i$ $2\times8n$
[2] $P\bar{4}2c$ (112)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2b;2d$	$2a;2c$	$4m$ $2\times4m$	$2e;2f$ $4k;4l$	$4h;4j$ $8n$	$4g;4i$ $2\times8n$
Enlarged unit cell, isomorphic								
[3] $P\bar{4}c2$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4g$	$2b;4h$	$2c;4g$ $3\times4g$	$2d;4h$ $3\times4h$	$4f;8j$ $3\times4i$	$4e;8j$ $3\times8j$
[p] $P\bar{4}c2$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ p = prime >2;	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $u=1,\dots,p-1$	$2a;\frac{p-1}{2}\times4g$	$2b;\frac{p-1}{2}\times4h$	$2c;\frac{p-1}{2}\times4g$ $p\times4g$	$2d;\frac{p-1}{2}\times4h$ $p\times4h$	$4e(f^*);\frac{p-1}{2}\times8j$ $p\times4i$	$4f(e^*);\frac{p-1}{2}\times8j$ $p\times8j$
[9] $P\bar{4}c2$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4e;4f;8j$	$2b;4e;4f;8j$	$2c;2\times8j$ $4g;4\times8j$	$2d;2\times8j$ $4h;4\times8j$	$3\times4e;3\times8j$ $4i;4\times8j$	$3\times4f;3\times8j$ $9\times8j$
[p^2] $P\bar{4}c2$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ p = prime >2;	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\dots,p-1$	$2a;\frac{p-1}{2}\times4e;$ $\frac{p-1}{2}\times4f;$ $\frac{(p-1)^2}{4}\times8j$	$2b;\frac{p-1}{2}\times4e;$ $\frac{p-1}{2}\times4f;$ $\frac{(p-1)^2}{4}\times8j$	$2c;\frac{p^2-1}{4}\times8j$ $4g;\frac{p^2-1}{2}\times8j$	$2d;\frac{p^2-1}{4}\times8j$ $4h;\frac{p^2-1}{2}\times8j$	$p\times4e;\frac{p(p-1)}{2}\times8j$ $4i;\frac{p^2-1}{2}\times8j$	$p\times4f;\frac{p(p-1)}{2}\times8j$ $p^2\times8j$

$^*p=4n-1$

D_{2d}^{7} No. 117 $P\bar{4}b2$

	Axes	Coordinates	Wyckoff positions					
			2*a*	2*b*	2*c*	2*d* 4*g*	4*e* 4*h*	4*f* 8*i*
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}$ (81)			1*a*; 1*c*	1*b*; 1*d*	2*g*	2*g* 4*h*	2*e*; 2*f* 4*h*	2×2*g* 2×4*h*
[2] *Pba*2 (32)			2*a*	2*a*	2*b*	2*b* 4*c*	2×2*a* 4*c*	2×2*b* 2×4*c*
[2] *C*222 (21)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z$;	4*k*	4*k*	2*a*; 2*b*	2*c*; 2*d* 4*e*; 4*g*	2×4*k* 4*f*; 4*h*	4*i*; 4*j* 2×8*l*
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P\bar{4}n2$ (118)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*a*; 2*b*	4*e*	4*h*	2*c*; 2*d* 8*i*	2×4*e* 4*f*; 4*g*	2×4*h* 2×8*i*
[2] $P\bar{4}n2$ (118)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*e*	2*a*; 2*b*	2*c*; 2*d*	4*h* 4*f*; 4*g*	2×4*e* 8*i*	2×4*h* 2×8*i*
Enlarged unit cell, isomorphic								
[2] $P\bar{4}b2$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*a*; 2*b*	4*e*	2*c*; 2*d*	4*f* 4*g*; 4*h*	2×4*e* 8*i*	2×4*f* 2×8*i*
[2] $P\bar{4}b2$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	4*e*	2*a*; 2*b*	4*f*	2*c*; 2*d* 8*i*	2×4*e* 4*g*; 4*h*	2×4*f* 2×8*i*
[3] $P\bar{4}b2$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$;	2*a*; 4*e*	2*b*; 4*e*	2*c*; 4*f*	2*d*; 4*f* 4*g*; 8*i*	3×4*e* 4*h*; 8*i*	3×4*f* 3×8*i*
[*p*] $P\bar{4}b2$	**a**, **b**, *p***c** *p* = prime > 2;	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $u = 1, \ldots, p-1$	2*a*; $\frac{p-1}{2}$×4*e*	2*b*; $\frac{p-1}{2}$×4*e*	2*c*; $\frac{p-1}{2}$×4*f*	2*d*; $\frac{p-1}{2}$×4*f* 4*g*; $\frac{p-1}{2}$×8*i*	*p*×4*e* 4*h*; $\frac{p-1}{2}$×8*i*	*p*×4*f* *p*×8*i*
[9] $P\bar{4}b2$	3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	2*a*; 2×8*i*	2*b*; 2×8*i*	2*c*; 2×4*g*; 8*i*	2*d*; 2×4*h*; 8*i* 3×4*g*; 3×8*i*	4*e*; 4×8*i* 3×4*h*; 3×8*i*	4*f*; 4×8*i* 9×8*i*
[p^2] $P\bar{4}b2$	*p***a**, *p***b**, **c** *p* = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ $u, v = 1, \ldots, p-1$	2*a*; $\frac{p^2-1}{4}$×8*i*	2*b*; $\frac{p^2-1}{4}$×8*i*	2*c*; (*p*−1)×4*g*; $\frac{(p-1)^2}{4}$×8*i*	2*d*; (*p*−1)×4*h*; $\frac{(p-1)^2}{4}$×8*i* *p*×4*g*; $\frac{p(p-1)}{2}$×8*i*	4*e*; $\frac{p^2-1}{2}$×8*i* *p*×4*h*; $\frac{p(p-1)}{2}$×8*i*	4*f*; $\frac{p^2-1}{2}$×8*i* p^2×8*i*

$P\bar{4}n2$ No. 118 D_{2d}^{8}

Subgroup	Axes	Coordinates	Wyckoff positions $2a$	$2b$	$2c$	$2d$ $4g$	$4e$ $4h$	$4f$ $8i$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}$ (81)			$1a; 1d$	$1b; 1c$	$2g$	$2g$ $4h$	$2e; 2f$ $2{\times}2g$	$4h$ $2{\times}4h$
[2] $Pnn2$ (34)			$2a$	$2a$	$2b$	$2b$ $4c$	$2{\times}2a$ $2{\times}2b$	$4c$ $2{\times}4c$
[2] $C222$ (21)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z+\frac{1}{4}$	$4k$	$4k$	$2a; 2c$	$2b; 2d$ $4e; 4h$	$2{\times}4k$ $4i; 4j$	$4f; 4g$ $2{\times}8l$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $I\bar{4}2d$ (122)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a; 4b$	$8c$	$8d$	$8d$ $16e$	$2{\times}8c$ $16e$	$2{\times}8d$ $2{\times}16e$
[2] $I\bar{4}2d$ (122)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y)$, $\frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$8c$	$4a; 4b$	$8d$	$8d$ $2{\times}8d$	$2{\times}8c$ $16e$	$16e$ $2{\times}16e$
[2] $I\bar{4}2d$ (122)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$8c$	$4a; 4b$	$8d$	$8d$ $16e$	$2{\times}8c$ $16e$	$2{\times}8d$ $2{\times}16e$
[2] $I\bar{4}2d$ (122)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y)$, $\frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$4a; 4b$	$8c$	$8d$	$8d$ $2{\times}8d$	$2{\times}8c$ $16e$	$16e$ $2{\times}16e$
Enlarged unit cell, isomorphic								
[3] $P\bar{4}n2$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a; 4e$	$2b; 4e$	$2d; 4h$	$2c; 4h$ $4f; 8i$	$3{\times}4e$ $3{\times}4h$	$4g; 8i$ $3{\times}8i$
[p] $P\bar{4}n2$ p = prime > 2;	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $u = 1, \ldots, p-1$	$2a; \frac{p-1}{2}{\times}4e$	$2b; \frac{p-1}{2}{\times}4e$	$2c(d^*); \frac{p-1}{2}{\times}4h$	$2d(c^*); \frac{p-1}{2}{\times}4h$ $4g(f^*); \frac{p-1}{2}{\times}8i$	$p{\times}4e$ $p{\times}4h$	$4f(g^*); \frac{p-1}{2}{\times}8i$ $p{\times}8i$
[9] $P\bar{4}n2$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$2a; 2{\times}8i$	$2b; 2{\times}8i$	$2c; 4f; 4g; 8i$	$2d; 4f; 4g; 8i$ $3{\times}4g; 3{\times}8i$	$4e; 4{\times}8i$ $4h; 4{\times}8i$	$3{\times}4f; 3{\times}8i$ $9{\times}8i$
[p^2] $P\bar{4}n2$ p = prime > 2;	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$ $u, v = 1, \ldots, p-1$	$2a; \frac{p^2-1}{4}{\times}8i$	$2b; \frac{p^2-1}{4}{\times}8i$	$2c; \frac{p-1}{2}{\times}4f$; $\frac{p-1}{2}{\times}4g$; $\frac{(p-1)^2}{4}{\times}8i$	$2d; \frac{p-1}{2}{\times}4f$; $\frac{p-1}{2}{\times}4g$; $\frac{(p-1)^2}{4}{\times}8i$ $p{\times}4g; \frac{p(p-1)}{2}{\times}8i$	$4e; \frac{p^2-1}{2}{\times}8i$ $4h; \frac{p^2-1}{2}{\times}8i$	$p{\times}4f; \frac{p(p-1)}{2}{\times}8i$ $p^2{\times}8i$

$^*\, p = 4n-1$

D_{2d}^9 No. 119 $I\bar{4}m2$

Axes	Coordinates	Wyckoff positions					
		$2a$	$2b$	$2c$ $8g$	$2d$ $8h$	$4e$ $8i$	$4f$ $16j$
I Maximal *translationengleiche* subgroups							
[2] $I\bar{4}$ (82)		$2a$	$2b$	$2c$ $8g$	$2d$ $8g$	$4e$ $8g$	$4f$ $2\times 8g$
[2] $Imm2$ (44)		$2a$	$2a$	$2b$ $8e$	$2b$ $8e$	$2\times 2a$ $4c; 4d$	$2\times 2b$ $2\times 8e$
[2] $F222$ (22) **a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$4a$	$4b$	$4d$ $8e; 8f$	$4c$ $8i; 8j$	$8g$ $16k$	$8h$ $2\times 16k$
II Maximal *klassengleiche* subgroups							
Loss of centring translations							
[2] $P\bar{4}n2$ (118)		$2a$	$2b$	$2c$ $8i$	$2d$ $4f; 4g$	$4e$ $8i$	$4h$ $2\times 8i$
[2] $P\bar{4}n2$ (118)	$x+\frac{1}{2}, y, z+\frac{1}{4}$	$2d$	$2c$	$2a$ $4f; 4g$	$2b$ $8i$	$4h$ $8i$	$4e$ $2\times 8i$
[2] $P\bar{4}m2$ (115)		$1a; 1c$	$1b; 1d$	$2g$ $4h; 4i$	$2g$ $8l$	$2e; 2f$ $4j; 4k$	$2\times 2g$ $2\times 8l$
[2] $P\bar{4}m2$ (115)	$x+\frac{1}{2}, y, z+\frac{1}{4}$	$2g$	$2g$	$1a; 1c$ $8l$	$1b; 1d$ $4h; 4i$	$2\times 2g$ $4j; 4k$	$2e; 2f$ $2\times 8l$
Enlarged unit cell, isomorphic							
[3] $I\bar{4}m2$ **a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$2a; 4e$	$2b; 4e$	$2d; 4f$ $8g; 16j$	$2c; 4f$ $8h; 16j$	$3\times 4e$ $3\times 8i$	$3\times 4f$ $3\times 16j$
[p] $I\bar{4}m2$ **a**, **b**, p**c** p = prime > 2;	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$ $u = 1, \ldots, p-1$	$2a; \frac{p-1}{2}\times 4e$	$2b; \frac{p-1}{2}\times 4e$	$2c(d^*); \frac{p-1}{2}\times 4f$ $8g; \frac{p-1}{2}\times 16j$	$2d(c^*); \frac{p-1}{2}\times 4f$ $8h; \frac{p-1}{2}\times 16j$	$p\times 4e$ $p\times 8i$	$p\times 4f$ $p\times 16j$
[9] $I\bar{4}m2$ 3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z;$ $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$2a; 8g; 8i$	$2b; 8g; 8i$	$2c; 8h; 8i$ $3\times 8g; 3\times 16j$	$2d; 8h; 8i$ $3\times 8h; 3\times 16j$	$4e; 2\times 8i; 16j$ $3\times 8i; 3\times 16j$	$4f; 2\times 8i; 16j$ $9\times 16j$
[p^2] $I\bar{4}m2$ p**a**, p**b**, **c** p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$ $u, v = 1, \ldots, p-1$	$2a; \frac{p-1}{2}\times 8g;$ $\frac{p-1}{2}\times 8i;$ $\frac{(p-1)(p-3)}{8}\times 16j$	$2b; \frac{p-1}{2}\times 8g;$ $\frac{p-1}{2}\times 8i;$ $\frac{(p-1)(p-3)}{8}\times 16j$	$2c; \frac{p-1}{2}\times 8h;$ $\frac{p-1}{2}\times 8i;$ $\frac{(p-1)(p-3)}{8}\times 16j$ $p\times 8g;$ $\frac{p(p-1)}{2}\times 16j$	$2d; \frac{p-1}{2}\times 8h;$ $\frac{p-1}{2}\times 8i;$ $\frac{(p-1)(p-3)}{8}\times 16j$ $p\times 8h;$ $\frac{p(p-1)}{2}\times 16j$	$4e; (p-1)\times 8i;$ $\frac{(p-1)^2}{4}\times 16j$ $p\times 8i;$ $\frac{p(p-1)}{2}\times 16j$	$4f; (p-1)\times 8i;$ $\frac{(p-1)^2}{4}\times 16j$ $p^2\times 16j$

$^*\ p = 4n-1$

$I\bar{4}c2$ No. 120 D_{2d}^{10}

	Axes	Coordinates	Wyckoff positions					
			$4a$	$4b$	$4c$	$4d$ $8g$	$8e$ $8h$	$8f$ $16i$
I Maximal *translationengleiche* subgroups								
[2] $I\bar{4}$ (82)			$4e$	$2a;2b$	$2c;2d$	$4f$ $2\times4f$	$8g$ $8g$	$2\times4e$ $2\times8g$
[2] $Iba2$ (45)			$4a$	$4a$	$4b$	$4b$ $2\times4b$	$8c$ $8c$	$2\times4a$ $2\times8c$
[2] $F222$ (22)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z+\frac{1}{4}$	$4a;4b$	$8g$	$8h$	$4c;4d$ $2\times8h$	$8e;8f$ $8i;8j$	$2\times8g$ $2\times16k$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P\bar{4}b2$ (117)			$4e$	$2a;2b$	$4f$	$2c;2d$ $2\times4f$	$8i$ $4g;4h$	$2\times4e$ $2\times8i$
[2] $P\bar{4}b2$ (117)		$x+\frac{1}{2}, y, z+\frac{1}{4}$	$2c;2d$	$4f$	$2a;2b$	$4e$ $2\times4e$	$4g;4h$ $8i$	$2\times4f$ $2\times8i$
[2] $P\bar{4}c2$ (116)			$2a;2b$	$2c;2d$	$4i$	$4i$ $2\times4i$	$4e;4f$ $8j$	$4g;4h$ $2\times8j$
[2] $P\bar{4}c2$ (116)		$x+\frac{1}{2}, y, z+\frac{1}{4}$	$4i$	$4i$	$2c;2d$	$2a;2b$ $4g;4h$	$8j$ $4e;4f$	$2\times4i$ $2\times8j$
Enlarged unit cell, isomorphic								
[3] $I\bar{4}c2$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a;8f$	$4b;8f$	$4c;8g$	$4d;8g$ $3\times8g$	$8e;16i$ $8h;16i$	$3\times8f$ $3\times16i$
[p] $I\bar{4}c2$	**a**, **b**, p**c** p = prime > 2;	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $u = 1,\ldots,p-1$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8f$	$4c;\frac{p-1}{2}\times8g$	$4d;\frac{p-1}{2}\times8g$ $p\times8g$	$8e;\frac{p-1}{2}\times16i$ $8h;\frac{p-1}{2}\times16i$	$p\times8f$ $p\times16i$
[9] $I\bar{4}c2$	3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$4a;2\times8e;16i$	$4b;2\times16i$	$4c;2\times16i$	$4d;2\times8h;16i$ $8g;4\times16i$	$3\times8e;3\times16i$ $3\times8h;3\times16i$	$8f;4\times16i$ $9\times16i$
[p^2] $I\bar{4}c2$	p**a**, p**b**, **c** p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ $u,v = 1,\ldots,p-1$	$4a;(p-1)\times8e;$ $\frac{(p-1)^2}{4}\times16i$	$4b;\frac{p^2-1}{4}\times16i$	$4c;\frac{p^2-1}{4}\times16i$	$4d;(p-1)\times8h;$ $\frac{(p-1)^2}{4}\times16i$ $8g;\frac{p^2-1}{2}\times16i$	$p\times8e;$ $\frac{p(p-1)}{2}\times16i$ $p\times8h;$ $\frac{p(p-1)}{2}\times16i$	$8f;\frac{p^2-1}{2}\times16i$ $p^2\times16i$

D_{2d}^{11} No. 121 $I\bar{4}2m$

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$4c$ $8g$	$4d$ $8h$	$4e$ $8i$	$8f$ $16j$
I Maximal *translationengleiche* subgroups								
[2] $I\bar{4}$ (82)			$2a$	$2b$	$4f$ $8g$	$2c;2d$ $2\times4f$	$4e$ $8g$	$8g$ $2\times8g$
[2] $I222$ (23)			$2a$	$2c$	$2b;2d$ $4f;4h$	$4j$ $2\times4j$	$4i$ $8k$	$4e;4g$ $2\times8k$
[2] $Fmm2$ (42)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$4a$	$4a$	$8b$ $16e$	$8b$ $2\times8b$	$2\times4a$ $8c;8d$	$16e$ $2\times16e$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P\bar{4}2_1c$ (114)			$2a$	$2b$	$4d$ $8e$	$4d$ $2\times4d$	$4c$ $8e$	$8e$ $2\times8e$
[2] $P\bar{4}2_1m$ (113)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2c$	$2c$	$4d$ $8f$	$2a;2b$ $2\times4d$	$2\times2c$ $2\times4e$	$8f$ $2\times8f$
[2] $P\bar{4}2c$ (112)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2b$	$2d$	$2a;2c$ $4i;4j$	$2e;2f$ $4k;4l$	$4m$ $8n$	$4g;4h$ $2\times8n$
[2] $P\bar{4}2m$ (111)			$1a;1b$	$1c;1d$	$2e;2f$ $4k;4l$	$4m$ $2\times4m$	$2g;2h$ $2\times4n$	$4i;4j$ $2\times8o$
Enlarged unit cell, isomorphic								
[3] $I\bar{4}2m$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$4c;8h$ $8g;16j$	$4d;8h$ $3\times8h$	$3\times4e$ $3\times8i$	$8f;16j$ $3\times16j$
[p] $I\bar{4}2m$ p = prime >2;	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$4c;\frac{p-1}{2}\times8h$ $8g;\frac{p-1}{2}\times16j$	$4d;\frac{p-1}{2}\times8h$ $p\times8h$	$p\times4e$ $p\times8i$	$8f;\frac{p-1}{2}\times16j$ $p\times16j$
[9] $I\bar{4}2m$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;8f;8i$	$2b;8g;8i$	$4c;8f;8g;16j$ $3\times8g;3\times16j$	$4d;2\times16j$ $8h;4\times16j$	$4e;2\times8i;16j$ $3\times8i;3\times16j$	$3\times8f;3\times16j$ $9\times16j$
[p^2] $I\bar{4}2m$ p = prime >2;	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times8f;$ $\frac{p-1}{2}\times8i;$ $\frac{(p-1)(p-3)}{8}\times16j$	$2b;\frac{p-1}{2}\times8g;$ $\frac{p-1}{2}\times8i;$ $\frac{(p-1)(p-3)}{8}\times16j$	$4c;\frac{p-1}{2}\times8f;$ $\frac{p-1}{2}\times8g;$ $\frac{(p-1)^2}{4}\times16j$ $p\times8g;$ $\frac{p(p-1)}{2}\times16j$	$4d;\frac{p^2-1}{4}\times16j$ $8h;\frac{p^2-1}{2}\times16j$	$4e;(p-1)\times8i;$ $\frac{(p-1)^2}{4}\times16j$ $p\times8i;$ $\frac{p(p-1)}{2}\times16j$	$p\times8f;$ $\frac{p(p-1)}{2}\times16j$ $p^2\times16j$

$I\bar{4}2d$ No. 122 D_{2d}^{12}

	Axes	Coordinates	Wyckoff positions				
			$4a$	$4b$	$8c$	$8d$	$16e$
I Maximal *translationengleiche* subgroups							
[2] $I\bar{4}$ (82)			$2a; 2c$	$2b; 2d$	$4e; 4f$	$8g$	$2\times 8g$
[2] $I2_12_12_1$ (24)		$x, y+\frac{1}{4}, z+\frac{1}{8}$	$4c$	$4c$	$2\times 4c$	$4a; 4b$	$2\times 8d$
[2] $Fdd2$ (43)	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z$	$8a$	$8a$	$2\times 8a$	$16b$	$2\times 16b$
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[3] $I\bar{4}2d$	$\mathbf{b}, -\mathbf{a}, 3\mathbf{c}$	$y, -x, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$4a; 8c$	$4b; 8c$	$3\times 8c$	$8d; 16e$	$3\times 16e$
[p] $I\bar{4}2d$	$\mathbf{b}, -\mathbf{a}, p\mathbf{c}$	$y, -x, \frac{1}{p}z; +(0,0,\frac{u}{p})$ $p = \text{prime} = 4n-1;\ u = 1,\ldots,p-1$	$4a; \frac{p-1}{2}\times 8c$	$4b; \frac{p-1}{2}\times 8c$	$p\times 8c$	$8d; \frac{p-1}{2}\times 16e$	$p\times 16e$
[5] $I\bar{4}2d$	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$	$4a; 2\times 8c$	$4b; 2\times 8c$	$5\times 8c$	$8d; 2\times 16e$	$5\times 16e$
[p] $I\bar{4}2d$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$ $p = \text{prime} = 4n+1;\ u = 1,\ldots,p-1$	$4a; \frac{p-1}{2}\times 8c$	$4b; \frac{p-1}{2}\times 8c$	$p\times 8c$	$8d; \frac{p-1}{2}\times 16e$	$p\times 16e$
[9] $I\bar{4}2d$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$4a; 2\times 16e$	$4b; 2\times 16e$	$8c; 4\times 16e$	$3\times 8d; 3\times 16e$	$9\times 16e$
[p^2] $I\bar{4}2d$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$ $p = \text{prime} > 2;\ u,v = 1,\ldots,p-1$	$4a; \frac{p^2-1}{4}\times 16e$	$4b; \frac{p^2-1}{4}\times 16e$	$8c; \frac{p^2-1}{2}\times 16e$	$p\times 8d;$ $\frac{p(p-1)}{2}\times 16e$	$p^2\times 16e$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 123, pp. 599–601.

D_{4h}^{1} $P4/m2/m2/m$ No. 123 $P4/mmm$

	Axes	Coordinates	Wyckoff positions $1a$	 $1b$	 $1c$	 $1d$	 $2e$ $4l$	 $2f$ $4m$	 $2g$ $4n$	 $2h$ $4o$	 $4i$ $8p$ $8s$	 $4j$ $8q$ $8t$	 $4k$ $8r$ $16u$
I Maximal *translationengleiche* subgroups													
[2] $P\bar{4}m2$ (115)			$1a$	$1d$	$1b$	$1c$	$2g$ $4j$	$2g$ $4j$	$2e$ $4k$	$2f$ $4k$	$2{\times}2g$ $8l$ $2{\times}4j$	$4h$ $8l$ $2{\times}4k$	$4i$ $8l$ $2{\times}8l$
[2] $P\bar{4}2m$ (111)			$1a$	$1c$	$1d$	$1b$	$2f$ $4i$	$2e$ $4k$	$2g$ $4l$	$2h$ $4j$	$4m$ $8o$ $8o$	$4n$ $8o$ $8o$	$4n$ $2{\times}4n$ $2{\times}8o$
[2] $P4mm$ (99)			$1a$	$1a$	$1b$	$1b$	$2c$ $4e$	$2c$ $4e$	$2{\times}1a$ $4f$	$2{\times}1b$ $4f$	$2{\times}2c$ $8g$ $2{\times}4e$	$4d$ $8g$ $2{\times}4f$	$4d$ $2{\times}4d$ $2{\times}8g$
[2] $P422$ (89)			$1a$	$1b$	$1c$	$1d$	$2f$ $4l$	$2e$ $4n$	$2g$ $4o$	$2h$ $4m$	$4i$ $8p$ $8p$	$4j$ $8p$ $8p$	$4k$ $8p$ $2{\times}8p$
[2] $P4/m$ (83)			$1a$	$1b$	$1c$	$1d$	$2f$ $4j$	$2e$ $4k$	$2g$ $4j$	$2h$ $4k$	$4i$ $2{\times}4j$ $8l$	$4j$ $2{\times}4k$ $8l$	$4k$ $8l$ $2{\times}8l$
[2] $Pmmm$ (47)			$1a$	$1c$	$1f$	$1h$	$1d$; $1g$ $2i$; $2m$	$1b$; $1e$ $2j$; $2n$	$2q$ $2k$; $2o$	$2t$ $2l$; $2p$	$2r$; $2s$ $2{\times}4y$ $4u$; $4w$	$4y$ $2{\times}4z$ $4v$; $4x$	$4z$ 8α $2{\times}8\alpha$
[2] $Cmmm$ (65)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2a$	$2d$	$2b$	$2c$	$4f$ $8p$	$4e$ $8q$	$4k$ $8p$	$4l$ $8q$	$8m$ $2{\times}8p$ $16r$	$4g$; $4i$ $2{\times}8q$ $16r$	$4h$; $4j$ $8n$; $8o$ $2{\times}16r$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**													
[2] $I4/mcm$ (140)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4c$	$4a$	$4d$	$4b$	$8e$ $16k$	$8h$ $16i$	$8f$ $2{\times}8h$	$8g$ $16l$	$16l$ $2{\times}16k$ $32m$	$16k$ $32m$ $2{\times}16l$	$16j$ $32m$ $2{\times}32m$
[2] $I4/mcm$ (140)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4a$	$4c$	$4b$	$4d$	$8h$ $16i$	$8e$ $16k$	$8f$ $16l$	$8g$ $2{\times}8h$	$16l$ $32m$ $32m$	$16j$ $2{\times}16k$ $2{\times}16l$	$16k$ $32m$ $2{\times}32m$
[2] $I4/mcm$ (140)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4d$	$4b$	$4c$	$4a$	$8e$ $2{\times}8h$	$8h$ $16l$	$8g$ $16k$	$8f$ $16i$	$16l$ $2{\times}16k$ $2{\times}16l$	$16k$ $32m$ $32m$	$16j$ $32m$ $2{\times}32m$
[2] $I4/mcm$ (140)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4b$	$4d$	$4a$	$4c$	$8h$ $16l$	$8e$ $2{\times}8h$	$8g$ $16i$	$8f$ $16k$	$16l$ $32m$ $2{\times}16l$	$16j$ $2{\times}16k$ $32m$	$16k$ $32m$ $2{\times}32m$
[2] $I4/mmm$ (139)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a$; $2b$	$4e$	$4c$	$4d$	$8f$ $2{\times}8h$	$8h$ $16m$	$2{\times}4e$ $16l$	$8g$ $16k$	$16m$ $2{\times}16l$ $2{\times}16m$	$8i$; $8j$ $32o$ $32o$	$16n$ $2{\times}16n$ $2{\times}32o$
[2] $I4/mmm$ (139)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4e$	$2a$; $2b$	$4d$	$4c$	$8h$ $16m$	$8f$ $2{\times}8h$	$2{\times}4e$ $16k$	$8g$ $16l$	$16m$ $32o$ $2{\times}16m$	$16n$ $2{\times}16l$ $32o$	$8i$; $8j$ $2{\times}16n$ $2{\times}32o$

	Axes	Coordinates	Wyckoff positions 1*a*	 1*b*	 1*c*	 1*d*	 2*e* 4*l*	 2*f* 4*m*	 2*g* 4*n*	 2*h* 4*o*	 4*i* 8*p* 8*s*	 4*j* 8*q* 8*t*	 4*k* 8*r* 16*u*
[2] $I4/mmm$ (139)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z;$ $+(0,0,\frac{1}{2})$	4*c*	4*d*	2*a*; 2*b*	4*e*	8*f* 16*l*	8*h* 16*k*	8*g* 2×8*h*	2×4*e* 16*m*	16*m* 2×16*l* 32*o*	8*i*; 8*j* 32*o* 2×16*m*	16*n* 2×16*n* 2×32*o*
[2] $I4/mmm$ (139)	**a**−**b**, **a**+**b**, 2**c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), \frac{1}{2}z+\frac{1}{4};$ $+(0,0,\frac{1}{2})$	4*d*	4*c*	4*e*	2*a*; 2*b*	8*h* 16*k*	8*f* 16*l*	8*g* 16*m*	2×4*e* 2×8*h*	16*m* 32*o* 32*o*	16*n* 2×16*l* 2×16*m*	8*i*; 8*j* 2×16*n* 2×32*o*
[2] $P4_2/mcm$ (132)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2*a*	2*b*	2*c*	2*d*	4*e* 8*n*	4*f* 8*l*	4*g* 8*n*	4*h* 8*m*	8*k* 2×8*n* 16*p*	4*i*; 4*j* 16*p* 16*p*	8*o* 2×8*o* 2×16*p*
[2] $P4_2/mcm$ (132)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	2*b*	2*a*	2*d*	2*c*	4*f* 8*l*	4*e* 8*n*	4*g* 8*m*	4*h* 8*n*	8*k* 16*p* 16*p*	8*o* 2×8*n* 16*p*	4*i*; 4*j* 2×8*o* 2×16*p*
[2] $P4_2/mmc$ (131)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2*a*	2*e*	2*b*	2*f*	4*i* 4*j*; 4*l*	2*c*; 2*d* 8*o*	4*g* 4*k*; 4*m*	4*h* 8*p*	2×4*i* 2×8*q* 2×8*o*	8*q* 16*r* 2×8*p*	8*n* 16*r* 2×16*r*
[2] $P4_2/mmc$ (131)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	2*e*	2*a*	2*f*	2*b*	2*c*; 2*d* 8*o*	4*i* 4*j*; 4*l*	4*g* 8*p*	4*h* 4*k*; 4*m*	2×4*i* 16*r* 2×8*o*	8*n* 2×8*q* 2×8*p*	8*q* 16*r* 2×16*r*
[2] $P4/nmm$ (129)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	2*a*	2*b*	2*c*	2*c*	4*e* 8*g*	4*d* 8*h*	4*f* 8*j*	2×2*c* 8*j*	8*j* 16*k* 16*k*	8*i* 16*k* 2×8*j*	8*i* 2×8*i* 2×16*k*
[2] $P4/nmm$ (129)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	2*c*	2*c*	2*a*	2*b*	4*e* 8*j*	4*d* 8*j*	2×2*c* 8*g*	4*f* 8*h*	8*j* 16*k* 2×8*j*	8*i* 16*k* 16*k*	8*i* 2×8*i* 2×16*k*
[2] $P4/mbm$ (127)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z;$ $+(\frac{1}{2},\frac{1}{2},0)$	2*a*	2*b*	2*d*	2*c*	4*h* 8*i*	4*g* 8*j*	4*e* 2×4*g*	4*f* 2×4*h*	8*k* 2×8*i* 16*l*	8*i* 2×8*j* 2×8*k*	8*j* 16*l* 2×16*l*
[2] $P4/mbm$ (127)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z;$ $+(\frac{1}{2},\frac{1}{2},0)$	2*d*	2*c*	2*a*	2*b*	4*h* 2×4*g*	4*g* 2×4*h*	4*f* 8*i*	4*e* 8*j*	8*k* 2×8*i* 2×8*k*	8*i* 2×8*j* 16*l*	8*j* 16*l* 2×16*l*
[2] $P4/nbm$ (125)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	2*a*	2*b*	2*c*	2*d*	4*f* 8*i*	4*e* 8*j*	4*g* 8*m*	4*h* 8*m*	8*m* 16*n* 16*n*	8*k* 16*n* 2×8*m*	8*l* 16*n* 2×16*n*
[2] $P4/nbm$ (125)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y), z; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	2*c*	2*d*	2*a*	2*b*	4*f* 8*m*	4*e* 8*m*	4*h* 8*i*	4*g* 8*j*	8*m* 16*n* 2×8*m*	8*k* 16*n* 16*n*	8*l* 16*n* 2×16*n*
[2] $P4/mcc$ (124)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2*b*	2*a*	2*d*	2*c*	4*f* 8*m*	4*e* 8*k*	4*g* 8*m*	4*h* 8*l*	8*i* 2×8*m* 16*n*	8*m* 16*n* 16*n*	8*j* 16*n* 2×16*n*
[2] $P4/mcc$ (124)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	2*a*	2*b*	2*c*	2*d*	4*e* 8*k*	4*f* 8*m*	4*g* 8*l*	4*h* 8*m*	8*i* 16*n* 16*n*	8*j* 2×8*m* 16*n*	8*m* 16*n* 2×16*n*

	Axes	Coordinates	Wyckoff positions					
			$1a$ $2g$	$1b$ $2h$ $4m$	$1c$ $4i$ $4n$ $8r$	$1d$ $4j$ $4o$ $8s$	$2e$ $4k$ $8p$ $8t$	$2f$ $4l$ $8q$ $16u$
Enlarged unit cell, isomorphic								
[2] $P4/mmm$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a$; $1b$ $2{\times}2g$	$2g$ $2{\times}2h$ $8s$	$1c$; $1d$ $2{\times}4i$ $4n$; $4o$ $2{\times}8r$	$2h$ $4j$; $4k$ $8t$ $2{\times}8s$	$4i$ $8r$ $8p$; $8q$ $2{\times}8t$	$2e$; $2f$ $4l$; $4m$ $16u$ $2{\times}16u$
[2] $P4/mmm$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2g$ $2{\times}2g$	$1a$; $1b$ $2{\times}2h$ $4l$; $4m$	$2h$ $2{\times}4i$ $8t$ $2{\times}8r$	$1c$; $1d$ $8r$ $4n$; $4o$ $2{\times}8s$	$2e$; $2f$ $4j$; $4k$ $16u$ $2{\times}8t$	$4i$ $8s$ $8p$; $8q$ $2{\times}16u$
[3] $P4/mmm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a$; $2g$ $3{\times}2g$	$1b$; $2g$ $3{\times}2h$ $4m$; $8s$	$1c$; $2h$ $3{\times}4i$ $4n$; $8t$ $3{\times}8r$	$1d$; $2h$ $4j$; $8r$ $4o$; $8t$ $3{\times}8s$	$2e$; $4i$ $4k$; $8r$ $8p$; $16u$ $3{\times}8t$	$2f$; $4i$ $4l$; $8s$ $8q$; $16u$ $3{\times}16u$
[p] $P4/mmm$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p =$ prime > 2; $u = 1,\ldots,p-1$	$1a$; $\frac{p-1}{2}{\times}2g$ $p{\times}2g$	$1b$; $\frac{p-1}{2}{\times}2g$ $p{\times}2h$ $4m$; $\frac{p-1}{2}{\times}8s$	$1c$; $\frac{p-1}{2}{\times}2h$ $p{\times}4i$ $4n$; $\frac{p-1}{2}{\times}8t$ $p{\times}8r$	$1d$; $\frac{p-1}{2}{\times}2h$ $4j$; $\frac{p-1}{2}{\times}8r$ $4o$; $\frac{p-1}{2}{\times}8t$ $p{\times}8s$	$2e$; $\frac{p-1}{2}{\times}4i$ $4k$; $\frac{p-1}{2}{\times}8r$ $8p$; $\frac{p-1}{2}{\times}16u$ $p{\times}8t$	$2f$; $\frac{p-1}{2}{\times}4i$ $4l$; $\frac{p-1}{2}{\times}8s$ $8q$; $\frac{p-1}{2}{\times}16u$ $p{\times}16u$
[2] $P4/mmm$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a$; $1c$ $2g$; $2h$	$1b$; $1d$ $4i$ $2{\times}4k$	$2f$ $8r$ $8p$ $8s$; $8t$	$2e$ $4l$; $4n$ $8q$ $2{\times}8r$	$4k$ $4m$; $4o$ $2{\times}8p$ $16u$	$4j$ $2{\times}4j$ $2{\times}8q$ $2{\times}16u$
[2] $P4/mmm$	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y), z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2f$ $4i$	$2e$ $2g$; $2h$ $8q$	$1a$; $1c$ $8r$ $2{\times}4j$ $8s$; $8t$	$1b$; $1d$ $4l$; $4n$ $2{\times}4k$ $16u$	$4k$ $4m$; $4o$ $2{\times}8p$ $2{\times}8r$	$4j$ $8p$ $2{\times}8q$ $2{\times}16u$
[9] $P4/mmm$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a$; $4j$; $4l$ $2g$; $8r$; $8s$	$1b$; $4k$; $4m$ $2h$; $8r$; $8t$ $3{\times}4m$; $3{\times}8q$	$1c$; $4j$; $4n$ $4i$; $8s$; $8t$; $16u$ $3{\times}4n$; $3{\times}8p$ $3{\times}8r$; $3{\times}16u$	$1d$; $4k$; $4o$ $3{\times}4j$; $3{\times}8p$ $3{\times}4o$; $3{\times}8q$ $3{\times}8s$; $3{\times}16u$	$2e$; $4m$; $4o$; $8q$ $3{\times}4k$; $3{\times}8q$ $9{\times}8p$ $3{\times}8t$; $3{\times}16u$	$2f$; $4l$; $4n$; $8p$ $3{\times}4l$; $3{\times}8p$ $9{\times}8q$ $9{\times}16u$
[p^2] $P4/mmm$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ $p =$ prime > 2; $u, v = 1,\ldots,p-1$	$1a$; $\frac{p-1}{2}{\times}4j$; $\frac{p-1}{2}{\times}4l$; $\frac{(p-1)(p-3)}{8}{\times}8p$ $2g$; $\frac{p-1}{2}{\times}8r$; $\frac{p-1}{2}{\times}8s$; $\frac{(p-1)(p-3)}{8}{\times}16u$	$1b$; $\frac{p-1}{2}{\times}4k$; $\frac{p-1}{2}{\times}4m$; $\frac{(p-1)(p-3)}{8}{\times}8q$ $2h$; $\frac{p-1}{2}{\times}8r$; $\frac{p-1}{2}{\times}8t$; $\frac{(p-1)(p-3)}{8}{\times}16u$ $p{\times}4m$; $\frac{p(p-1)}{2}{\times}8q$	$1c$; $\frac{p-1}{2}{\times}4j$; $\frac{p-1}{2}{\times}4n$; $\frac{(p-1)(p-3)}{8}{\times}8p$ $4i$; $\frac{p-1}{2}{\times}8s$; $\frac{p-1}{2}{\times}8t$; $\frac{(p-1)^2}{4}{\times}16u$ $p{\times}4n$; $\frac{p(p-1)}{2}{\times}8p$ $p{\times}8r$; $\frac{p(p-1)}{2}{\times}16u$	$1d$; $\frac{p-1}{2}{\times}4k$; $\frac{p-1}{2}{\times}4o$; $\frac{(p-1)(p-3)}{8}{\times}8q$ $p{\times}4j$; $\frac{p(p-1)}{2}{\times}8p$ $p{\times}4o$; $\frac{p(p-1)}{2}{\times}8q$ $p{\times}8s$; $\frac{p(p-1)}{2}{\times}16u$	$2e$; $\frac{p-1}{2}{\times}4m$; $\frac{p-1}{2}{\times}4o$; $\frac{(p-1)^2}{4}{\times}8q$ $p{\times}4k$; $\frac{p(p-1)}{2}{\times}8q$ $p^2{\times}8p$ $p{\times}8t$; $\frac{p(p-1)}{2}{\times}16u$	$2f$; $\frac{p-1}{2}{\times}4l$; $\frac{p-1}{2}{\times}4n$; $\frac{(p-1)^2}{4}{\times}8p$ $p{\times}4l$; $\frac{p(p-1)}{2}{\times}8p$ $p^2{\times}8q$ $p^2{\times}16u$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 124, pp. 602–603.

$P4/mcc$ No. 124 $P4/m\,2/c\,2/c$ D_{4h}^{2}

	Axes	Coordinates	2a	2b	2c	2d	4e	4f	4g	4h	8i 8l	8j 8m	8k 16n
I Maximal *translationengleiche* subgroups													
[2] $P\bar{4}c2$ (116)			2a	2c	2b	2d	4i	4i	4g	4h	2×4i 8j	4e;4f 8j	8j 2×8j
[2] $P\bar{4}2c$ (112)			2a	2e	2c	2f	4m	2b;2d	4k	4l	2×4m 4h;4i	8n 8n	4g;4j 2×8n
[2] $P4cc$ (103)			2a	2a	2b	2b	4c	4c	2×2a	2×2b	2×4c 8d	8d 8d	8d 2×8d
[2] $P422$ (89)		$x,y,z+\frac{1}{4}$	1a;1b	2g	1c;1d	2h	4i	2e;2f	2×2g	2×2h	2×4i 4m;4o	4j;4k 8p	4l;4n 2×8p
[2] $P4/m$ (83)			2g	1a;1b	2h	1c;1d	2e;2f	4i	2×2g	2×2h	2×4i 8l	8l 4j;4k	8l 2×8l
[2] $Pccm$ (49)			2e	2a	2h	2b	2c;2d	2f;2g	4m	4n	4o;4p 4j;4l	8r 2×4q	4i;4k 2×8r
[2] $Cccm$ (66)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	4a	4c	4b	4d	4e;4f	8k	8i	8j	2×8k 16m	8g;8h 2×8l	16m 2×16m
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**													
[2] $P4/ncc$ (130)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z;+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	4a	4b	4c	4c	8d	8f	8e	2×4c	16g 16g	16g 16g	2×8f 2×16g
[2] $P4/ncc$ (130)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y),z;+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	4c	4c	4a	4b	8d	8f	2×4c	8e	16g 2×8f	16g 16g	16g 2×16g
[2] $P4/mnc$ (128)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	4e	2a;2b	4d	4c	8h	8g	2×4e	8f	16i 2×8g	16i 2×8h	16i 2×16i
[2] $P4/mnc$ (128)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	4d	4c	4e	2a;2b	8h	8g	8f	2×4e	16i 16i	16i 2×8h	2×8g 2×16i
[2] $P4/nnc$ (126)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	2a;2b	4e	4c	4d	8f	8h	2×4e	8g	16k 16k	8i;8j 16k	2×8h 2×16k
[2] $P4/nnc$ (126)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	4c	4d	2a;2b	4e	8f	8h	8g	2×4e	16k 2×8h	8i;8j 16k	16k 2×16k

Axes	Coordinates	Wyckoff positions					
		$2a$	$2b$ $4g$	$2c$ $4h$	$2d$ $8i$ $8l$	$4e$ $8j$ $8m$	$4f$ $8k$ $16n$
Enlarged unit cell, isomorphic							
[3] $P4/mcc$ $\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4g$	$2b;4g$ $3\times4g$	$2c;4h$ $3\times4h$	$2d;4h$ $3\times8i$ $8l;16n$	$4e;8i$ $8j;16n$ $8m;16n$	$4f;8i$ $8k;16n$ $3\times16n$
[p] $P4/mcc$ $\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=$ prime >2;	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4g$	$2b;\frac{p-1}{2}\times4g$ $p\times4g$	$2c;\frac{p-1}{2}\times4h$ $p\times4h$	$2d;\frac{p-1}{2}\times4h$ $p\times8i$ $8l;\frac{p-1}{2}\times16n$	$4e;\frac{p-1}{2}\times8i$ $8j;\frac{p-1}{2}\times16n$ $8m;\frac{p-1}{2}\times16n$	$4f;\frac{p-1}{2}\times8i$ $8k;\frac{p-1}{2}\times16n$ $p\times16n$
[2] $P4/mcc$ $\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2c$	$2b;2d$ $4g;4h$	$4f$ $8i$	$4e$ $16n$ $16n$	$8m$ $8k;8l$ $2\times8m$	$8j$ $2\times8j$ $2\times16n$
[2] $P4/mcc$ $\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y),z$; $+(\frac{1}{2},\frac{1}{2},0)$	$4f$	$4e$ $8i$	$2a;2c$ $4g;4h$	$2b;2d$ $16n$ $2\times8j$	$8m$ $8k;8l$ $2\times8m$	$8j$ $16n$ $2\times16n$
[9] $P4/mcc$ $3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z$; $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;8j;8k$	$2b;2\times8m$ $4g;2\times16n$	$2c;8j;8l$ $4h;2\times16n$	$2d;2\times8m$ $8i;4\times16n$ $3\times8l;3\times16n$	$4e;4\times8m$ $3\times8j;3\times16n$ $9\times8m$	$4f;8k;8l;16n$ $3\times8k;3\times16n$ $9\times16n$
[p^2] $P4/mcc$ $p\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=$ prime >2;	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times8j$; $\frac{p-1}{2}\times8k$; $\frac{(p-1)(p-3)}{8}\times16n$	$2b;\frac{p^2-1}{4}\times8m$ $4g;\frac{p^2-1}{4}\times16n$	$2c;\frac{p-1}{2}\times8j$; $\frac{p-1}{2}\times8l$; $\frac{(p-1)(p-3)}{8}\times16n$ $4h;\frac{p^2-1}{4}\times16n$	$2d;\frac{p^2-1}{4}\times8m$ $8i;\frac{p^2-1}{2}\times16n$ $p\times8l$; $\frac{p(p-1)}{2}\times16n$	$4e;\frac{p^2-1}{2}\times8m$ $p\times8j$; $\frac{p(p-1)}{2}\times16n$ $p^2\times8m$	$4f;\frac{p-1}{2}\times8k$; $\frac{p-1}{2}\times8l$; $\frac{(p-1)^2}{4}\times16n$ $p\times8k$; $\frac{p(p-1)}{2}\times16n$ $p^2\times16n$

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$P4/nbm$ No. 125 $P4/n2/b2/m$ D_{4h}^{3}

I Maximal *translationengleiche* subgroups

	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$8i$ $8l$	$8j$ $8m$	$8k$ $16n$
[2] $P\bar{4}b2$ (117)		$x+\frac{1}{2},y,z$	$x+\frac{1}{4},y-\frac{1}{4},z$	$2c$	$2d$	$2a$	$2b$	$4g$	$4h$	$4f$	$4e$	$2\times4g$ $8i$	$2\times4h$ $8i$	$8i$ $2\times8i$
[2] $P\bar{4}2m$ (111)		$x+\frac{1}{2},y,z$	$x+\frac{1}{4},y-\frac{1}{4},z$	$2e$	$2f$	$1a;1d$	$1b;1c$	$4n$	$4n$	$4m$	$2g;2h$	$8o$ $4j;4k$	$8o$ $2\times4n$	$4i;4l$ $2\times8o$
[2] $P4bm$ (100)			$x+\frac{1}{4},y+\frac{1}{4},z$	$2a$	$2a$	$2b$	$2b$	$4c$	$4c$	$2\times2a$	$2\times2b$	$8d$ $8d$	$8d$ $2\times4c$	$8d$ $2\times8d$
[2] $P422$ (89)			$x+\frac{1}{4},y+\frac{1}{4},z$	$1a;1c$	$1b;1d$	$2e$	$2f$	$4j$	$4k$	$2g;2h$	$4i$	$2\times4j$ $4m;4n$	$2\times4k$ $8p$	$4l;4o$ $2\times8p$
[2] $P4/n$ (85)		$x+\frac{1}{2},y,z$		$2c$	$2c$	$2a$	$2b$	$4d$	$4e$	$2\times2c$	$4f$	$8g$ $8g$	$8g$ $8g$	$8g$ $2\times8g$
[2] $Pban$ (50)				$2a$	$2d$	$2b$	$2c$	$4e$	$4f$	$4k$	$4l$	$8m$ $4h;4j$	$8m$ $8m$	$4g;4i$ $2\times8m$
[2] $Cmme$ (67)	**a**+**b**, −**a**+**b**, **c**	$\frac{1}{2}(x+y)+\frac{1}{4}$, $\frac{1}{2}(-x+y),z$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),z$	$4a$	$4b$	$4g$	$4g$	$4c;4e$	$4d;4f$	$8l$	$2\times4g$	$8h;8j$ $16o$	$8i;8k$ $8m;8n$	$16o$ $2\times16o$

II Maximal *klassengleiche* subgroups
Enlarged unit cell, non-isomorphic

	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$8i$ $8l$	$8j$ $8m$	$8k$ $16n$
[2] $P4_2/nnm$ (134)	**a**, **b**, 2**c**	$x+\frac{1}{2},y,\frac{1}{2}z+\frac{1}{4}$	$x,y,\frac{1}{2}z$	$4d$	$4c$	$4g$	$2a;2b$	$4e;4f$	$8m$	$8h$	$2\times4g$	$8k;8l$ $8i;8j$	$16n$ $2\times8m$	$16n$ $2\times16n$
[2] $P4_2/nnm$ (134)	**a**, **b**, 2**c**	$x+\frac{1}{2},y,\frac{1}{2}z$	$x,y,\frac{1}{2}z+\frac{1}{4}$	$4c$	$4d$	$2a;2b$	$4g$	$8m$	$4e;4f$	$8h$	$2\times4g$	$16n$ $16n$	$8k;8l$ $2\times8m$	$8i;8j$ $2\times16n$
[2] $P4_2/nbc$ (133)	**a**, **b**, 2**c**	$x+\frac{1}{2},y,\frac{1}{2}z+\frac{1}{4}$	$x,y,\frac{1}{2}z$	$4a$	$4c$	$4b$	$4d$	$8e$	$8j$	$8f$	$8g$	$16k$ $16k$	$2\times8j$ $16k$	$8h;8i$ $2\times16k$
[2] $P4_2/nbc$ (133)	**a**, **b**, 2**c**	$x+\frac{1}{2},y,\frac{1}{2}z$	$x,y,\frac{1}{2}z+\frac{1}{4}$	$4c$	$4a$	$4d$	$4b$	$8j$	$8e$	$8f$	$8g$	$2\times8j$ $8h;8i$	$16k$ $16k$	$16k$ $2\times16k$
[2] $P4/nnc$ (126)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4}$	$x,y,\frac{1}{2}z$	$4e$	$2a;2b$	$4d$	$4c$	$8f$	$8h$	$2\times4e$	$8g$	$16k$ $8i;8j$	$2\times8h$ $16k$	$16k$ $2\times16k$
[2] $P4/nnc$ (126)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z$	$x,y,\frac{1}{2}z+\frac{1}{4}$	$2a;2b$	$4e$	$4c$	$4d$	$8h$	$8f$	$2\times4e$	$8g$	$2\times8h$ $16k$	$16k$ $16k$	$8i;8j$ $2\times16k$

	Axes	Coordinates origin 1	origin 2	Wyckoff positions $2a$	$2b$	$2c$	$2d$	$4e$
				$4f$	$4g$	$4h$	$8i$	$8j$
					$8k$	$8l$	$8m$	$16n$
Enlarged unit cell, isomorphic								
[2] $P4/nbm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;$	$x,y,\frac{1}{2}z;$	$2a;2b$	$4g$	$2c;2d$	$4h$	$4e;4f$
		$\pm(0,0,\frac{1}{2})$	$\pm(0,0,\frac{1}{2})$	$8m$	$2\times4g$	$2\times4h$	$8i;8j$	$16n$
					$8k;8l$	$16n$	$2\times8m$	$2\times16n$
[2] $P4/nbm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};$	$x,y,\frac{1}{2}z+\frac{1}{4};$	$4g$	$2a;2b$	$4h$	$2c;2d$	$8m$
		$\pm(0,0,\frac{1}{2})$	$\pm(0,0,\frac{1}{2})$	$4e;4f$	$2\times4g$	$2\times4h$	$16n$	$8i;8j$
					$16n$	$8k;8l$	$2\times8m$	$2\times16n$
[3] $P4/nbm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;$	$x,y,\frac{1}{3}z;$	$2a;4g$	$2b;4g$	$2c;4h$	$2d;4h$	$4e;8m$
		$\pm(0,0,\frac{1}{3})$	$\pm(0,0,\frac{1}{3})$	$4f;8m$	$3\times4g$	$3\times4h$	$8i;16n$	$8j;16n$
					$8k;16n$	$8l;16n$	$3\times8m$	$3\times16n$
[p] $P4/nbm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;$	$x,y,\frac{1}{p}z;$	$2a;\frac{p-1}{2}\times4g$	$2b;\frac{p-1}{2}\times4g$	$2c;\frac{p-1}{2}\times4h$	$2d;\frac{p-1}{2}\times4h$	$4e;\frac{p-1}{2}\times8m$
		$+(0,0,\frac{u}{p})$	$+(0,0,\frac{u}{p})$	$4f;\frac{p-1}{2}\times8m$	$p\times4g$	$p\times4h$	$8i;\frac{p-1}{2}\times16n$	$8j;\frac{p-1}{2}\times16n$
	$p=\text{prime}>2;\ u=1,\ldots,p-1$				$8k;\frac{p-1}{2}\times16n$	$8l;\frac{p-1}{2}\times16n$	$p\times8m$	$p\times16n$
[9] $P4/nbm$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$	$\frac{1}{3}x,\frac{1}{3}y,z;$	$2a;8i;8k;$	$2b;8j;8l$	$2c;8k;8m$	$2d;8l;8m$	$4e;8i;8m;16n$
		$\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$		$4f;8j;8m;16n$	$4g;2\times16n$	$4h;2\times8m;16n$	$3\times8i;3\times16n$	$3\times8j;3\times16n$
		$\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$			$3\times8k;3\times16n$	$3\times8l;3\times16n$	$3\times8m;3\times16n$	$9\times16n$
[p^2] $P4/nbm$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;$ $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x,\frac{1}{p}y,z;$ $+(\frac{u}{p},\frac{v}{p},0)$	$2a;\frac{p-1}{2}\times8i;$ $\frac{p-1}{2}\times8k;$ $\frac{(p-1)(p-3)}{8}\times16n$	$2b;\frac{p-1}{2}\times8j;$ $\frac{p-1}{2}\times8l;$ $\frac{(p-1)(p-3)}{8}\times16n$	$2c;\frac{p-1}{2}\times8k;$ $\frac{p-1}{2}\times8m;$ $\frac{(p-1)(p-3)}{8}\times16n$	$2d;\frac{p-1}{2}\times8l;$ $\frac{p-1}{2}\times8m;$ $\frac{(p-1)(p-3)}{8}\times16n$	$4e;\frac{p-1}{2}\times8i;$ $\frac{p-1}{2}\times8m;$ $\frac{(p-1)^2}{4}\times16n$
	$p=\text{prime}>2;$	$u,v=1,\ldots,p-1$		$4f;\frac{p-1}{2}\times8j;$ $\frac{p-1}{2}\times8m;$ $\frac{(p-1)^2}{4}\times16n$	$4g;\frac{p^2-1}{4}\times16n$	$4h;(p-1)\times8m;$ $\frac{(p-1)^2}{4}\times16n$	$p\times8i;$ $\frac{p(p-1)}{2}\times16n$	$p\times8j;$ $\frac{p(p-1)}{2}\times16n$
					$p\times8k;$ $\frac{p(p-1)}{2}\times16n$	$p\times8l;$ $\frac{p(p-1)}{2}\times16n$	$p\times8m;$ $\frac{p(p-1)}{2}\times16n$	$p^2\times16n$

$P4/nnc$ No. 126 $P4/n2/n2/c$ D_{4h}^4

Subgroup	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions 2a	2b 8g	4c 8h	4d 8i	4e 8j	8f 16k
I Maximal *translationengleiche* subgroups									
[2] $P\bar{4}n2$ (118)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$x+\frac{1}{4},y-\frac{1}{4},z$	$2d$	$2c$ $2\times4e$	$4e$ $4f;4g$	$2a;2b$ $8i$	$4h$ $8i$	$8i$ $2\times8i$
[2] $P\bar{4}2c$ (112)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$x+\frac{1}{4},y-\frac{1}{4},z$	$2b$	$2d$ $4k;4l$	$2a;2c$ $8n$	$2e;2f$ $4g;4h$	$4m$ $4i;4j$	$8n$ $2\times8n$
[2] $P4nc$ (104)			$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$2a$	$2a$ $2\times4b$	$4b$ $8c$	$4b$ $8c$	$2\times2a$ $8c$	$8c$ $2\times8c$
[2] $P422$ (89)			$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$1a;1d$	$1b;1c$ $2\times4i$	$2e;2f$ $4j;4k$	$4i$ $4l;4m$	$2g;2h$ $4n;4o$	$8p$ $2\times8p$
[2] $P4/n$ (85)		$x+\frac{1}{2},y,z+\frac{1}{4}$		$2c$	$2c$ $2\times4f$	$4f$ $8g$	$2a;2b$ $8g$	$2\times2c$ $8g$	$4d;4e$ $2\times8g$
[2] $Pnnn$ (48)				$2a$	$2c$ $2\times4l$	$2b;2d$ $8m$	$4l$ $4g;4i$	$4k$ $4h;4j$	$4e;4f$ $2\times8m$
[2] $Ccce$ (68)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$4a$	$4b$ $2\times8h$	$8h$ $8e;8f$	$8h$ $16i$	$8g$ $16i$	$8c;8d$ $2\times16i$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, isomorphic									
[3] $P4/nnc$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$2a(b^*);4e$	$2b(a^*);4e$ $3\times8g$	$4c;8g$ $8h;16k$	$4d;8g$ $8i(j^*);16k$	$3\times4e$ $8j(i^*);16k$	$8f;16k$ $3\times16k$
[p] $P4/nnc$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$2a(b^\dagger);\frac{p-1}{2}\times4e$	$2b(a^\dagger);\frac{p-1}{2}\times4e$ $p\times8g$	$4c;\frac{p-1}{2}\times8g$ $8h;\frac{p-1}{2}\times16k$	$4d;\frac{p-1}{2}\times8g$ $8i(j^\dagger);\frac{p-1}{2}\times16k$	$p\times4e$ $8j(i^\dagger);\frac{p-1}{2}\times16k$	$8f;\frac{p-1}{2}\times16k$ $p\times16k$
	p = prime; $u=1,\ldots,p-1$								
[9] $P4/nnc$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a(b^*);8h;8i(j^*)$	$2b(a^*);8h;8j(i^*)$ $8g;4\times16k$	$4c;8i;8j;16k$ $3\times8h;3\times16k$	$4d;2\times16k$ $3\times8i(j^*);3\times16k$	$4e;2\times16k$ $3\times8j(i^*);3\times16k$	$8f;4\times16k$ $9\times16k$
[p^2] $P4/nnc$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$2a(b^\dagger);\frac{p-1}{2}\times8h;$ $\frac{p-1}{2}\times8i(j^\dagger);$ $\frac{(p-1)(p-3)}{8}\times16k$	$2b(a^\dagger);\frac{p-1}{2}\times8h;$ $\frac{p-1}{2}\times8j(i^\dagger);$ $\frac{(p-1)(p-3)}{8}\times16k$ $8g;\frac{p^2-1}{2}\times16k$	$4c;\frac{p-1}{2}\times8i;$ $\frac{p-1}{2}\times8j;$ $\frac{(p-1)^2}{4}\times16k$ $p\times8h;$ $\frac{p(p-1)}{2}\times16k$	$4d;$ $\frac{p^2-1}{4}\times16k$ $p\times8i(j^\dagger);$ $\frac{p(p-1)}{2}\times16k$	$4e;$ $\frac{p^2-1}{4}\times16k$ $p\times8j(i^\dagger);$ $\frac{p(p-1)}{2}\times16k$	$8f;$ $\frac{p^2-1}{4}\times16k$ $p^2\times16k$
	p = prime >2; $u,v=1,\ldots,p-1$								

* origin 2

† origin 2 and $p=4n-1$

D_{4h}^{5} $P4/m2_1/b2/m$ No. 127 $P4/mbm$

	Axes	Coordinates	Wyckoff positions											
			$2a$	$2b$	$2c$	$2d$	$4e$	$4f$	$4g$	$4h$	$8i$	$8j$	$8k$	$16l$
I Maximal *translationengleiche* subgroups														
[2] $P\bar{4}b2$ (117)			$2a$	$2b$	$2d$	$2c$	$4e$	$4f$	$4g$	$4h$	$8i$	$8i$	$8i$	$2\times8i$
[2] $P\bar{4}2_1m$ (113)			$2a$	$2b$	$2c$	$2c$	$4d$	$2\times2c$	$4e$	$4e$	$8f$	$8f$	$2\times4e$	$2\times8f$
[2] $P4bm$ (100)			$2a$	$2a$	$2b$	$2b$	$2\times2a$	$2\times2b$	$4c$	$4c$	$8d$	$8d$	$2\times4c$	$2\times8d$
[2] $P42_12$ (90)		$x+\frac{1}{2},y,z$	$2c$	$2c$	$2b$	$2a$	$2\times2c$	$4d$	$4e$	$4f$	$8g$	$8g$	$8g$	$2\times8g$
[2] $P4/m$ (83)			$1a;1c$	$1b;1d$	$2f$	$2e$	$2g;2h$	$4i$	$4j$	$4k$	$2\times4j$	$2\times4k$	$8l$	$2\times8l$
[2] $Pbam$ (55)			$2a$	$2b$	$2d$	$2c$	$4e$	$4f$	$4g$	$4h$	$2\times4g$	$2\times4h$	$8i$	$2\times8i$
[2] $Cmmm$ (65)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z$	$4e$	$4f$	$2c;2d$	$2a;2b$	$8m$	$4k;4l$	$4g;4i$	$4h;4j$	$2\times8p$	$2\times8q$	$8n;8o$	$2\times16r$
II Maximal *klassengleiche* subgroups														
Enlarged unit cell, non-isomorphic														
[2] $P4_2/mnm$ (136)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{2},y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4c$	$4d$	$4e$	$2a;2b$	$8h$	$2\times4e$	$4f;4g$	$8j$	$2\times8i$	$16k$	$2\times8j$	$2\times16k$
[2] $P4_2/mnm$ (136)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x+\frac{1}{2},y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4d$	$4c$	$2a;2b$	$4e$	$8h$	$2\times4e$	$8j$	$4f;4g$	$16k$	$2\times8i$	$2\times8j$	$2\times16k$
[2] $P4_2/mbc$ (135)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$4a$	$4b$	$4d$	$4c$	$8e$	$8f$	$8h$	$8g$	$2\times8h$	$16i$	$16i$	$2\times16i$
[2] $P4_2/mbc$ (135)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4b$	$4a$	$4c$	$4d$	$8e$	$8f$	$8g$	$8h$	$16i$	$2\times8h$	$16i$	$2\times16i$
[2] $P4/mnc$ (128)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2a;2b$	$4e$	$4d$	$4c$	$2\times4e$	$8f$	$8h$	$8g$	$2\times8h$	$16i$	$16i$	$2\times16i$
[2] $P4/mnc$ (128)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4e$	$2a;2b$	$4c$	$4d$	$2\times4e$	$8f$	$8g$	$8h$	$16i$	$2\times8h$	$16i$	$2\times16i$
Enlarged unit cell, isomorphic														
[2] $P4/mbm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;+(0,0,\frac{1}{2})$	$2a;2b$	$4e$	$4f$	$2c;2d$	$2\times4e$	$2\times4f$	$4g;4h$	$8k$	$8i;8j$	$16l$	$2\times8k$	$2\times16l$
[2] $P4/mbm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4e$	$2a;2b$	$2c;2d$	$4f$	$2\times4e$	$2\times4f$	$8k$	$4g;4h$	$16l$	$8i;8j$	$2\times8k$	$2\times16l$
[3] $P4/mbm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$2c;4f$	$2d;4f$	$3\times4e$	$3\times4f$	$4g;8k$	$4h;8k$	$8i;16l$	$8j;16l$	$3\times8k$	$3\times16l$

	Axes	Coordinates	Wyckoff positions					
			$2a$ $4g$	$2b$ $4h$	$2c$ $8i$	$2d$ $8j$	$4e$ $8k$	$4f$ $16l$
[p] $P4/mbm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$; $p=$ prime >2; $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4e$; $4g;\frac{p-1}{2}\times8k$	$2b;\frac{p-1}{2}\times4e$; $4h;\frac{p-1}{2}\times8k$	$2c;\frac{p-1}{2}\times4f$; $8i;\frac{p-1}{2}\times16l$	$2d;\frac{p-1}{2}\times4f$; $8j;\frac{p-1}{2}\times16l$	$p\times4e$; $p\times8k$	$p\times4f$; $p\times16l$
[9] $P4/mbm$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z$; $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times8i$; $3\times4g;3\times8i$	$2b;2\times8j$; $3\times4h;3\times8j$	$2c;2\times4h;8j$; $9\times8i$	$2d;2\times4g;8i$; $9\times8j$	$4e;2\times16l$; $3\times8k;3\times16l$	$4f;2\times8k;16l$; $9\times16l$
[p^2] $P4/mbm$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$; $p=$ prime >2; $u,v=1,\ldots,p-1$	$2a;\frac{p^2-1}{4}\times8i$; $p\times4g;\frac{p(p-1)}{2}\times8i$	$2b;\frac{p^2-1}{4}\times8j$; $p\times4h;\frac{p(p-1)}{2}\times8j$	$2c;(p-1)\times4h;\frac{(p-1)^2}{4}\times8j$; $p^2\times8i$	$2d;(p-1)\times4g;\frac{(p-1)^2}{4}\times8i$; $p^2\times8j$	$4e;\frac{p^2-1}{4}\times16l$; $p\times8k;\frac{p(p-1)}{2}\times16l$	$4f;(p-1)\times8k;\frac{(p-1)^2}{4}\times16l$; $p^2\times16l$

$P4/mnc$ No. 128 $P4/m2_1/n2/c$ D_{4h}^{6}

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$4c$	$4d$ $8g$	$4e$ $8h$	$8f$ $16i$

I Maximal *translationengleiche* subgroups

	Axes	Coordinates	$2a$	$2b$	$4c$	$4d$ / $8g$	$4e$ / $8h$	$8f$ / $16i$
[2] $P\bar{4}n2$ (118)			$2a$	$2b$	$4h$	$2c;2d$ $4f;4g$	$4e$ $8i$	$2\times4h$ $2\times8i$
[2] $P\bar{4}2_1c$ (114)			$2a$	$2b$	$4d$	$4d$ $8e$	$4c$ $8e$	$2\times4d$ $2\times8e$
[2] $P4nc$ (104)			$2a$	$2a$	$4b$	$4b$ $8c$	$2\times2a$ $8c$	$2\times4b$ $2\times8c$
[2] $P42_12$ (90)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2c$	$2c$	$4d$	$2a;2b$ $4e;4f$	$2\times2c$ $8g$	$2\times4d$ $2\times8g$
[2] $P4/m$ (83)			$1a;1d$	$1b;1c$	$2e;2f$	$4i$ $8l$	$2g;2h$ $4j;4k$	$2\times4i$ $2\times8l$
[2] $Pnnm$ (58)			$2a$	$2b$	$2c;2d$	$4f$ $8h$	$4e$ $2\times4g$	$2\times4f$ $2\times8h$
[2] $Cccm$ (66)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z$	$4e$	$4f$	$4c;4d$	$4a;4b$ $8g;8h$	$8k$ $2\times8l$	$8i;8j$ $2\times16m$

II Maximal *klassengleiche* subgroups

Enlarged unit cell, isomorphic

	Axes	Coordinates	$2a$	$2b$	$4c$	$4d$ / $8g$	$4e$ / $8h$	$8f$ / $16i$
[3] $P4/mnc$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$	$4c;8f$	$4d;8f$ $8g;16i$	$3\times4e$ $8h;16i$	$3\times8f$ $3\times16i$
[p] $P4/mnc$ p = prime >2	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$	$4c;\frac{p-1}{2}\times8f$	$4d;\frac{p-1}{2}\times8f$ $8g;\frac{p-1}{2}\times16i$	$p\times4e$ $8h;\frac{p-1}{2}\times16i$	$p\times8f$ $p\times16i$
[9] $P4/mnc$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z$; $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;2\times8h$	$2b;2\times8h$	$4c;4\times8h$	$4d;2\times8g;16i$ $3\times8g;3\times16i$	$4e;2\times16i$ $9\times8h$	$8f;4\times16i$ $9\times16i$
[p^2] $P4/mnc$ p = prime >2;	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a;\frac{p^2-1}{4}\times8h$	$2b;\frac{p^2-1}{4}\times8h$	$4c;\frac{p^2-1}{2}\times8h$	$4d;(p-1)\times8g;\frac{(p-1)^2}{4}\times16i$ $p\times8g;\frac{p(p-1)}{2}\times16i$	$4e;\frac{p^2-1}{4}\times16i$ $p^2\times8h$	$8f;\frac{p^2-1}{2}\times16i$ $p^2\times16i$

D_{4h}^{7} $P4/n2_1/m2/m$ No. 129 $P4/nmm$

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions 2a	2b	2c	4d	4e	4f	8g	8h	8i	8j	16k
I Maximal *translationengleiche* subgroups														
[2] $P\bar{4}m2$ (115)			$x+\frac{1}{4},y-\frac{1}{4},z$	$1a;1b$	$1c;1d$	$2g$	$4h$	$4i$	$2e;2f$	$2\times4h$	$2\times4i$	$4j;4k$	$8l$	$2\times8l$
[2] $P\bar{4}2_1m$ (113)			$x+\frac{1}{4},y-\frac{1}{4},z$	$2a$	$2b$	$2c$	$4e$	$4e$	$4d$	$8f$	$8f$	$8f$	$2\times4e$	$2\times8f$
[2] $P4mm$ (99)		$x+\frac{1}{2},y,z$	$x-\frac{1}{4},y-\frac{1}{4},z$	$2c$	$2c$	$1a;1b$	$4d$	$4d$	$2\times2c$	$8g$	$8g$	$4e;4f$	$2\times4d$	$2\times8g$
[2] $P42_12$ (90)			$x+\frac{1}{4},y-\frac{1}{4},z$	$2a$	$2b$	$2c$	$4e$	$4f$	$4d$	$2\times4e$	$2\times4f$	$8g$	$8g$	$2\times8g$
[2] $P4/n$ (85)				$2a$	$2b$	$2c$	$4d$	$4e$	$4f$	$8g$	$8g$	$8g$	$8g$	$2\times8g$
[2] $Pmmn$ (59)				$2a(b^*)$	$2a(b^*)$	$2b(a^*)$	$4c$	$4d$	$2\times2a(b^*)$	$8g$	$8g$	$4e;4f$	$8g$	$2\times8g$
[2] $Cmme$ (67)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y),z$	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z$	$4a$	$4b$	$4g$	$4c;4e$	$4d;4f$	$8l$	$8h;8j$	$8i;8k$	$16o$	$8m;8n$	$2\times16o$
II Maximal *klassengleiche* subgroups														
Enlarged unit cell, non-isomorphic														
[2] $P4_2/ncm$ (138)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4b$	$4a$	$4e$	$8i$	$4c;4d$	$8f$	$16j$	$8g;8h$	$16j$	$2\times8i$	$2\times16j$
[2] $P4_2/ncm$ (138)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a$	$4b$	$4e$	$4c;4d$	$8i$	$8f$	$8g;8h$	$16j$	$16j$	$2\times8i$	$2\times16j$
[2] $P4_2/nmc$ (137)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2a;2b$	$4c$	$4d$	$8f$	$8e$	$2\times4c$	$2\times8f$	$16h$	$2\times8g$	$16h$	$2\times16h$
[2] $P4_2/nmc$ (137)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4c$	$2a;2b$	$4d$	$8e$	$8f$	$2\times4c$	$16h$	$2\times8f$	$2\times8g$	$16h$	$2\times16h$
[2] $P4/ncc$ (130)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4b$	$4a$	$4c$	$8d$	$8f$	$8e$	$16g$	$2\times8f$	$16g$	$16g$	$2\times16g$
[2] $P4/ncc$ (130)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4a$	$4b$	$4c$	$8f$	$8d$	$8e$	$2\times8f$	$16g$	$16g$	$16g$	$2\times16g$
Enlarged unit cell, isomorphic														
[2] $P4/nmm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a;2b$	$4f$	$2\times2c$	$4d;4e$	$8j$	$2\times4f$	$8g;8h$	$16k$	$2\times8i$	$2\times8j$	$2\times16k$
[2] $P4/nmm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4f$	$2a;2b$	$2\times2c$	$8j$	$4d;4e$	$2\times4f$	$16k$	$8g;8h$	$2\times8i$	$2\times8j$	$2\times16k$
[3] $P4/nmm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a;4f$	$2b;4f$	$3\times2c$	$4d;8j$	$4e;8j$	$3\times4f$	$8g;16k$	$8h;16k$	$3\times8i$	$3\times8j$	$3\times16k$

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions 2a	2b 4f	2c 8g	4d 8h 8j	4e 8i 16k
[p] $P4/nmm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4f$	$2b;\frac{p-1}{2}\times4f$; $p\times4f$	$p\times2c$; $8g;\frac{p-1}{2}\times16k$	$4d;\frac{p-1}{2}\times8j$; $8h;\frac{p-1}{2}\times16k$; $p\times8j$	$4e;\frac{p-1}{2}\times8j$; $p\times8i$; $p\times16k$
p = prime >2; $u=1,\dots p-1$								
[9] $P4/nmm$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\underbrace{\frac{1}{3}x,\frac{1}{3}y,z;\quad \frac{1}{3}x,\frac{1}{3}y,z;}$ $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$		$2a;8g;8i$	$2b;8h;8i$; $4f;2\times8i;16k$	$2c;8i;8j$; $3\times8g;3\times16k$	$4d;8g;8j;16k$; $3\times8h;\times16k$; $3\times8j;3\times16k$	$4e;8h;8j;16k$; $3\times8i;3\times16k$; $9\times16k$
[p^2] $P4/nmm$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a;\frac{p-1}{2}\times8g$; $\frac{p-1}{2}\times8i$; $\frac{(p-1)(p-3)}{8}\times16k$	$2b;\frac{p-1}{2}\times8h$; $\frac{p-1}{2}\times8i$; $\frac{(p-1)(p-3)}{8}\times16k$; $4f;(p-1)\times8i$; $\frac{(p-1)^2}{4}\times16k$	$2c;\frac{p-1}{2}\times8i$; $\frac{p-1}{2}\times8j$; $\frac{(p-1)(p-3)}{8}\times16k$; $p\times8g$; $\frac{p(p-1)}{2}\times16k$	$4d;\frac{p-1}{2}\times8g$; $\frac{p-1}{2}\times8j$; $\frac{(p-1)^2}{4}\times16k$; $p\times8h$; $\frac{p(p-1)}{2}\times16k$; $p\times8j$; $\frac{p(p-1)}{2}\times16k$	$4e;\frac{p-1}{2}\times8h$; $\frac{p-1}{2}\times8j$; $\frac{(p-1)^2}{4}\times16k$; $p\times8i$; $\frac{p(p-1)}{2}\times16k$; $p^2\times16k$
p = prime >2; $u,v=1,\dots p-1$								

* origin 2

$P4/ncc$ No. 130 $P4/n2_1/c2/c$ D_{4h}^{8}

	Axes	Coordinates origin 1	 origin 2	Wyckoff positions $4a$	 $4b$	 $4c$	 $8d$ $8f$	 $8e$ $16g$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}c2$ (116)			$x+\frac{1}{4}, y-\frac{1}{4}, z$	$2a; 2b$	$2c; 2d$	$4i$	$8j$ $4e; 4f$	$4g; 4h$ $2\times8j$
[2] $P\bar{4}2_1c$ (114)			$x+\frac{1}{4}, y-\frac{1}{4}, z$	$4c$	$2a; 2b$	$4d$	$8e$ $8e$	$2\times4c$ $2\times8e$
[2] $P4cc$ (103)		$x+\frac{1}{2}, y, z$	$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4c$	$4c$	$2a; 2b$	$8d$ $8d$	$2\times4c$ $2\times8d$
[2] $P42_12$ (90)		$x, y, z+\frac{1}{4}$	$x+\frac{1}{4}, y-\frac{1}{4},$ $z+\frac{1}{4}$	$2a; 2b$	$4d$	$2\times2c$	$8g$ $4e; 4f$	$2\times4d$ $2\times8g$
[2] $P4/n$ (85)				$4f$	$2a; 2b$	$2\times2c$	$4d; 4e$ $8g$	$2\times4f$ $2\times8g$
[2] $Pccn$ (56)		$x+\frac{1}{4}, y-\frac{1}{4}, z$		$4d$	$4d$	$4c$	$4a; 4b$ $8e$	$2\times4d$ $2\times8e$
[2] $Ccce$ (68)	**a**+**b**, −**a**+**b**, **c**	$\frac{1}{2}(x+y),$ $\frac{1}{2}(-x+y), z+\frac{1}{4}$	$\frac{1}{2}(x+y),$ $\frac{1}{2}(-x+y), z$	$4a; 4b$	$8g$	$8h$	$8c; 8d$ $8e; 8f$	$2\times8g$ $2\times16i$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**								
[3] $P4/ncc$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$x, y, \frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$4a; 8e$	$4b; 8e$	$3\times4c$	$8d; 16g$ $8f; 16g$	$3\times8e$ $3\times16g$
[p] $P4/ncc$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$x, y, \frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$4a; \frac{p-1}{2}\times8e$	$4b; \frac{p-1}{2}\times8e$	$p\times4c$	$8d; \frac{p-1}{2}\times16g$ $8f; \frac{p-1}{2}\times16g$	$p\times8e$ $p\times16g$
	p = prime > 2; $u = 1,\ldots,p-1$							
[9] $P4/ncc$	3**a**, 3**b**, **c**	$\frac{1}{3}x, \frac{1}{3}y, z;$	$\frac{1}{3}x, \frac{1}{3}y, z;$ $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0)$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$4a; 2\times8f; 16g$	$4b; 2\times16g$	$4c; 2\times16g$	$8d; 4\times16g$ $3\times8f; 3\times16g$	$8e; 4\times16g$ $9\times16g$
[p^2] $P4/ncc$	p**a**, p**b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z;$ $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x, \frac{1}{p}y, z;$ $+(\frac{u}{p},\frac{v}{p},0)$	$4a; (p-1)\times8f;$ $\frac{(p-1)^2}{4}\times16g$	$4b; \frac{p^2-1}{4}\times16g$	$4c; \frac{p^2-1}{4}\times16g$	$8d; \frac{p^2-1}{2}\times16g$ $p\times8f;$ $\frac{p(p-1)}{2}\times16g$	$8e; \frac{p^2-1}{2}\times16g$ $p^2\times16g$
	p = prime > 2; $u, v = 1,\ldots,p-1$							

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 131, pp. 611–612.

D_{4h}^{9} $P4_2/m2/m2/c$ No. 131 $P4_2/mmc$

	Axes	Coordinates	Wyckoff positions $2a$	 $2b$	 $2c$	 $2d$	 $2e$ $4l$	 $2f$ $4m$	 $4g$ $8n$	 $4h$ $8o$	 $4i$ $8p$	 $4j$ $8q$	 $4k$ $16r$
I Maximal *translationengleiche* subgroups													
[2] $P\bar{4}m2$ (115)		$x,y,z+\frac{1}{4}$	$2e$	$2f$	$2g$	$2g$	$1a;1d$ $4j$	$1b;1c$ $4k$	$2\times2e$ $4h;4i$	$2\times2f$ $2\times4j$	$2\times2g$ $2\times4k$	$4j$ $8l$	$4k$ $2\times8l$
[2] $P\bar{4}2c$ (112)		$x,y,z+\frac{1}{4}$	$2a$	$2c$	$2d$	$2b$	$2e$ $4j$	$2f$ $4i$	$4k$ $8n$	$4l$ $8n$	$4m$ $8n$	$4g$ $8n$	$4h$ $2\times8n$
[2] $P4_2mc$ (105)			$2a$	$2b$	$2c$	$2c$	$2a$ $4d$	$2b$ $4e$	$2\times2a$ $8f$	$2\times2b$ $2\times4d$	$2\times2c$ $2\times4e$	$4d$ $8f$	$4e$ $2\times8f$
[2] $P4_222$ (93)			$2a$	$2b$	$2c$	$2d$	$2e$ $4l$	$2f$ $4m$	$4g$ $4n;4o$	$4h$ $8p$	$4i$ $8p$	$4j$ $8p$	$4k$ $2\times8p$
[2] $P4_2/m$ (84)			$2a$	$2b$	$2c$	$2d$	$2e$ $4j$	$2f$ $4j$	$4g$ $8k$	$4h$ $8k$	$4i$ $8k$	$4j$ $2\times4j$	$4j$ $2\times8k$
[2] $Pmmm$ (47)			$1a;1c$	$1f;1h$	$1d;1e$	$1b;1g$	$2q$ $2j;2m$	$2t$ $2k;2p$	$2\times2q$ 8α	$2\times2t$ $4u;4w$	$2r;2s$ $4v;4x$	$2i;2n$ $4y;4z$	$2l;2o$ $2\times8\alpha$
[2] $Cccm$ (66)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z$	$4c$	$4d$	$4f$	$4e$	$4a$ $8l$	$4b$ $8l$	$8i$ $8g;8h$	$8j$ $16m$	$8k$ $16m$	$8l$ $2\times8l$	$8l$ $2\times16m$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**													
[2] $P4_2/ncm$ (138)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	$4a$	$4e$	$4d$	$4c$	$4b$ $8h$	$4e$ $8i$	$8f$ $16j$	$2\times4e$ $16j$	$8i$ $2\times8i$	$8g$ $16j$	$8i$ $2\times16j$
[2] $P4_2/ncm$ (138)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	$4e$	$4a$	$4c$	$4d$	$4e$ $8i$	$4b$ $8g$	$2\times4e$ $16j$	$8f$ $2\times8i$	$8i$ $16j$	$8i$ $16j$	$8h$ $2\times16j$
[2] $P4_2/mnm$ (136)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2b$	$4c$	$4g$	$4f$	$4e$ $2\times4g$	$4d$ $8i$	$2\times4e$ $16k$	$8h$ $2\times8j$	$8j$ $16k$	$2\times4f$ $2\times8i$	$8i$ $2\times16k$
[2] $P4_2/mnm$ (136)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4c$	$2a;2b$	$4f$	$4g$	$4d$ $8i$	$4e$ $2\times4f$	$8h$ $16k$	$2\times4e$ $16k$	$8j$ $2\times8j$	$8i$ $2\times8i$	$2\times4g$ $2\times16k$
[2] $P4_2/nnm$ (134)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	$4g$	$4d$	$4f$	$4e$	$2a;2b$ $8m$	$4c$ $8k$	$2\times4g$ $8i;8j$	$8h$ $2\times8m$	$8m$ $16n$	$8m$ $16n$	$8l$ $2\times16n$
[2] $P4_2/nnm$ (134)	**a**−**b**, **a**+**b**, **c**	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y),z+\frac{1}{4};+(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z;+(\frac{1}{2},\frac{1}{2},0)$	$4d$	$4g$	$4e$	$4f$	$4c$ $8l$	$2a;2b$ $8m$	$8h$ $8i;8j$	$2\times4g$ $16n$	$8m$ $2\times8m$	$8k$ $16n$	$8m$ $2\times16n$
[2] $P4_2/mcm$ (132)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2c$	$4f$	$4j$	$4i$	$2b;2d$ $2\times4j$	$4e$ $8n$	$4g;4h$ $8l;8m$	$8k$ $2\times8o$	$8o$ $16p$	$2\times4i$ $2\times8n$	$8n$ $2\times16p$
[2] $P4_2/mcm$ (132)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{2},\frac{1}{2}(x+y),z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4f$	$2a;2c$	$4i$	$4j$	$4e$ $8n$	$2b;2d$ $2\times4i$	$8k$ $8l;8m$	$4g;4h$ $16p$	$8o$ $2\times8o$	$8n$ $2\times8n$	$2\times4j$ $2\times16p$

	Axes	Coordinates	Wyckoff positions					
			$2a$ $4g$ $4m$	$2b$ $4h$ $8n$	$2c$ $4i$ $8o$	$2d$ $4j$ $8p$	$2e$ $4k$ $8q$	$2f$ $4l$ $16r$
Enlarged unit cell, isomorphic								
[3] $P4_2/mmc$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$2a; 4g$ $3\times 4g$ $4m; 8p$	$2b; 4h$ $3\times 4h$ $8n; 16r$	$2c; 4i$ $3\times 4i$ $3\times 8o$	$2d; 4i$ $4j; 8o$ $3\times 8p$	$2e; 4g$ $4k; 8p$ $8q; 16r$	$2f; 4h$ $4l; 8o$ $3\times 16r$
[p] $P4_2/mmc$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$ p = prime > 2; $u = 1, \ldots, p-1$	$2a; \frac{p-1}{2}\times 4g$ $p\times 4g$ $4m; \frac{p-1}{2}\times 8p$	$2b; \frac{p-1}{2}\times 4h$ $p\times 4h$ $8n; \frac{p-1}{2}\times 16r$	$2c; \frac{p-1}{2}\times 4i$ $p\times 4i$ $p\times 8o$	$2d; \frac{p-1}{2}\times 4i$ $4j; \frac{p-1}{2}\times 8o$ $p\times 8p$	$2e; \frac{p-1}{2}\times 4g$ $4k; \frac{p-1}{2}\times 8p$ $8q; \frac{p-1}{2}\times 16r$	$2f; \frac{p-1}{2}\times 4h$ $4l; \frac{p-1}{2}\times 8o$ $p\times 16r$
[9] $P4_2/mmc$	3**a**,3**b**,**c**	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3}, 0, 0)$; $\pm(0, \frac{1}{3}, 0)$; $\pm(\frac{1}{3}, \frac{1}{3}, 0)$; $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	$2a; 4j; 4l; 8q$ $4g; 2\times 8o; 16r$ $3\times 4m; 3\times 8q$	$2b; 4k; 4m; 8q$ $4h; 2\times 8p; 16r$ $3\times 8n; 3\times 16r$	$2c; 4l; 4m; 8q$ $4i; 8o; 8p; 16r$ $3\times 8o; 3\times 16r$	$2d; 4j; 4k; 8q$ $3\times 4j; 3\times 8q$ $3\times 8p; 3\times 16r$	$2e; 8n; 8o$ $3\times 4k; 3\times 8q$ $9\times 8q$	$2f; 8n; 8p$ $3\times 4l; 3\times 8q$ $9\times 16r$
[p^2] $P4_2/mmc$	p**a**,p**b**,**c**	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$ p = prime > 2; $u, v = 1, \ldots, p-1$	$2a; \frac{p-1}{2}\times 4j$; $\frac{p-1}{2}\times 4l$; $\frac{(p-1)^2}{4}\times 8q$ $4g; (p-1)\times 8o$; $\frac{(p-1)^2}{4}\times 16r$ $p\times 4m$; $\frac{p(p-1)}{2}\times 8q$	$2b; \frac{p-1}{2}\times 4k$; $\frac{p-1}{2}\times 4m$; $\frac{(p-1)^2}{4}\times 8q$ $4h; (p-1)\times 8p$; $\frac{(p-1)^2}{4}\times 16r$ $p\times 8n$; $\frac{p(p-1)}{2}\times 16r$	$2c; \frac{p-1}{2}\times 4l$; $\frac{p-1}{2}\times 4m$; $\frac{(p-1)^2}{4}\times 8q$ $4i; \frac{p-1}{2}\times 8o$; $\frac{p-1}{2}\times 8p$; $\frac{(p-1)^2}{4}\times 16r$ $p\times 8o$; $\frac{p(p-1)}{2}\times 16r$	$2d; \frac{p-1}{2}\times 4j$; $\frac{p-1}{2}\times 4k$; $\frac{(p-1)^2}{4}\times 8q$ $p\times 4j$; $\frac{p(p-1)}{2}\times 8q$ $p\times 8p$; $\frac{p(p-1)}{2}\times 16r$	$2e; \frac{p-1}{2}\times 8n$; $\frac{p-1}{2}\times 8o$; $\frac{(p-1)(p-3)}{8}\times 16r$ $p\times 4k$; $\frac{p(p-1)}{2}\times 8q$ $p^2\times 8q$	$2f; \frac{p-1}{2}\times 8n$; $\frac{p-1}{2}\times 8p$; $\frac{(p-1)(p-3)}{8}\times 16r$ $p\times 4l$; $\frac{p(p-1)}{2}\times 8q$ $p^2\times 16r$

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D_{4h}^{10} $P4_2/m2/c2/m$ No. 132 $P4_2/mcm$

	Axes	Coordinates	Wyckoff positions									
			$2a$	$2b$	$2c$	$2d$	$4e$ $8k$	$4f$ $8l$	$4g$ $8m$	$4h$ $8n$	$4i$ $8o$	$4j$ $16p$
I Maximal *translationengleiche* subgroups												
[2] $P\bar{4}c2$ (116)		$x,y,z+\frac{1}{4}$	$2a$	$2c$	$2b$	$2d$	$4i$ $2\times4i$	$4i$ $8j$	$4g$ $8j$	$4h$ $8j$	$4e$ $8j$	$4f$ $2\times8j$
[2] $P\bar{4}2m$ (111)		$x,y,z+\frac{1}{4}$	$2g$	$1a;1c$	$2h$	$1b;1d$	$2e;2f$ $2\times4m$	$4m$ $4i;4k$	$2\times2g$ $4j;4l$	$2\times2h$ $8o$	$4n$ $2\times4n$	$4n$ $2\times8o$
[2] $P4_2cm$ (101)			$2a$	$2a$	$2b$	$2b$	$4c$ $2\times4c$	$4c$ $8e$	$2\times2a$ $8e$	$2\times2b$ $8e$	$4d$ $2\times4d$	$4d$ $2\times8e$
[2] $P4_222$ (93)		$x,y,z+\frac{1}{4}$	$2e$	$2a$	$2f$	$2b$	$2c;2d$ $2\times4i$	$4i$ $4j;4l$	$4g$ $4k;4m$	$4h$ $8p$	$4n$ $8p$	$4o$ $2\times8p$
[2] $P4_2/m$ (84)			$2a$	$2e$	$2b$	$2f$	$4i$ $2\times4i$	$2c;2d$ $8k$	$4g$ $8k$	$4h$ $2\times4j$	$4j$ $8k$	$4j$ $2\times8k$
[2] $Pccm$ (49)			$2a$	$2e$	$2b$	$2h$	$2f;2g$ $4o;4p$	$2c;2d$ $4i;4k$	$4m$ $4j;4l$	$4n$ $2\times4q$	$4q$ $8r$	$4q$ $2\times8r$
[2] $Cmmm$ (65)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2a;2d$	$4k$	$2b;2c$	$4l$	$8m$ $2\times8m$	$4e;4f$ $16r$	$2\times4k$ $16r$	$2\times4l$ $8p;8q$	$4h;4i$ $8n;8o$	$4g;4j$ $2\times16r$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**												
[2] $P4_2/nmc$ (137)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z+\frac{1}{4}; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	$4c$	$2a;2b$	$4d$	$4d$	$8f$ $16h$	$8e$ $2\times8f$	$2\times4c$ $16h$	$2\times4d$ $16h$	$8g$ $2\times8g$	$8g$ $2\times16h$
[2] $P4_2/nmc$ (137)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y), z+\frac{1}{4}; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	$4d$	$4d$	$4c$	$2a;2b$	$8f$ $16h$	$8e$ $16h$	$2\times4d$ $2\times8f$	$2\times4c$ $16h$	$8g$ $2\times8g$	$8g$ $2\times16h$
[2] $P4_2/mbc$ (135)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4a$	$4b$	$4c$	$4d$	$8g$ $16i$	$8h$ $16i$	$8e$ $2\times8g$	$8f$ $2\times8h$	$8h$ $16i$	$8h$ $2\times16i$
[2] $P4_2/mbc$ (135)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$4c$	$4d$	$4a$	$4b$	$8g$ $16i$	$8h$ $2\times8g$	$8f$ $16i$	$8e$ $2\times8h$	$8h$ $16i$	$8h$ $2\times16i$
[2] $P4_2/nbc$ (133)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	origin 1: $\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z+\frac{1}{4}; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)-\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	$4b$	$4d$	$4a$	$4c$	$8j$ $16k$	$8e$ $16k$	$8g$ $2\times8j$	$8f$ $16k$	$8i$ $16k$	$8h$ $2\times16k$
[2] $P4_2/nbc$ (133)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	origin 1: $\frac{1}{2}(x-y)+\frac{1}{2}$, $\frac{1}{2}(x+y), z+\frac{1}{4}; +(\frac{1}{2},\frac{1}{2},0)$ origin 2: $\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z; +(\frac{1}{2},\frac{1}{2},0)$	$4a$	$4c$	$4b$	$4d$	$8j$ $16k$	$8e$ $2\times8j$	$8f$ $16k$	$8g$ $16k$	$8i$ $16k$	$8h$ $2\times16k$
[2] $P4_2/mmc$ (131)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2a;2b$	$2e;2f$	$2c;2d$	$4i$	$8n$ $16r$	$8q$ $2\times8n$	$4g;4h$ $16r$	$2\times4i$ $2\times8q$	$4k;4l$ $8o;8p$	$4j;4m$ $2\times16r$
[2] $P4_2/mmc$ (131)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{2}, \frac{1}{2}(x+y), z;$ $+(\frac{1}{2},\frac{1}{2},0)$	$2c;2d$	$4i$	$2a;2b$	$2e;2f$	$8n$ $16r$	$8q$ $16r$	$2\times4i$ $2\times8n$	$4g;4h$ $2\times8q$	$4k;4l$ $8o;8p$	$4j;4m$ $2\times16r$

Enlarged unit cell, isomorphic

	Axes	Coordinates	Wyckoff positions: $2a$ / $4g$	$2b$ / $4h$	$2c$ / $4i$ / $8m$	$2d$ / $4j$ / $8n$	$4e$ / $8k$ / $8o$	$4f$ / $8l$ / $16p$
[3] $P4_2/mcm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a;4g$ $3\times4g$	$2b;4g$ $3\times4h$	$2c;4h$ $4i;8o$ $8m;16p$	$2d;4h$ $4j;8o$ $8n;16p$	$4e;8k$ $3\times8k$ $3\times8o$	$4f;8k$ $8l;16p$ $3\times16p$
[p] $P4_2/mcm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4g$ $p\times4g$	$2b;\frac{p-1}{2}\times4g$ $p\times4h$	$2c;\frac{p-1}{2}\times4h$ $4i;\frac{p-1}{2}\times8o$ $8m;\frac{p-1}{2}\times16p$	$2d;\frac{p-1}{2}\times4h$ $4j;\frac{p-1}{2}\times8o$ $8n;\frac{p-1}{2}\times16p$	$4e;\frac{p-1}{2}\times8k$ $p\times8k$ $p\times8o$	$4f;\frac{p-1}{2}\times8k$ $8l;\frac{p-1}{2}\times16p$ $p\times16p$
[9] $P4_2/mcm$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4i;4j;8n$ $4g;2\times8o;16p$	$2b;8l;8o$ $4h;2\times8o;16p$	$2c;4i;4j;8n$ $3\times4i;3\times8n$ $3\times8m;3\times16p$	$2d;8m;8o$ $3\times4j;3\times8n$ $9\times8n$	$4e;8l;8m;16p$ $8k;4\times16p$ $3\times8o;3\times16p$	$4f;4\times8n$ $3\times8l;3\times16p$ $9\times16p$
[p^2] $P4_2/mcm$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$ $p=$ prime >2; $u,v=1,\ldots,p-1$	$2a;\frac{p-1}{2}\times4i;\frac{p-1}{2}\times4j;\frac{(p-1)^2}{4}\times8n$ $4g;(p-1)\times8o;\frac{(p-1)^2}{4}\times16p$	$2b;\frac{p-1}{2}\times8l;\frac{p-1}{2}\times8o;\frac{(p-1)(p-3)}{8}\times16p$ $4h;(p-1)\times8o;\frac{(p-1)^2}{4}\times16p$	$2c;\frac{p-1}{2}\times4i;\frac{p-1}{2}\times4j;\frac{(p-1)^2}{4}\times8n$ $p\times4i;\frac{p(p-1)}{2}\times8n$ $p\times8m;\frac{p(p-1)}{2}\times16p$	$2d;\frac{p-1}{2}\times8m;\frac{p-1}{2}\times8o;\frac{(p-1)(p-3)}{8}\times16p$ $p\times4j;\frac{p(p-1)}{2}\times8n$ $p^2\times8n$	$4e;\frac{p-1}{2}\times8l;\frac{p-1}{2}\times8m;\frac{(p-1)^2}{4}\times16p$ $8k;\frac{p^2-1}{2}\times16p$ $p\times8o;\frac{p(p-1)}{2}\times16p$	$4f;\frac{p^2-1}{2}\times8n$ $p\times8l;\frac{p(p-1)}{2}\times16p$ $p^2\times16p$

D_{4h}^{11} $P4_2/n2/b2/c$ No. 133 $P4_2/nbc$

	Axes	Coordinates origin 1	origin 2	Wyckoff positions 4a	4b 8g	4c 8h	4d 8i	8e 8j	8f 16k
I Maximal *translationengleiche* subgroups									
[2] $P\bar{4}b2$ (117)			$x+\frac{1}{4}$, $y-\frac{1}{4}, z+\frac{1}{4}$	$4f$	$4e$ $2\times4e$	$2c;2d$ $8i$	$2a;2b$ $8i$	$8i$ $4g;4h$	$2\times4f$ $2\times8i$
[2] $P\bar{4}2c$ (112)			$x+\frac{1}{4}$, $y-\frac{1}{4}, z+\frac{1}{4}$	$2b;2d$	$2a;2c$ $4k;4l$	$4m$ $4g;4i$	$2e;2f$ $4h;4j$	$8n$ $8n$	$2\times4m$ $2\times8n$
[2] $P4_2bc$ (106)		$x+\frac{1}{2}, y, z$	$x+\frac{1}{4}$, $y+\frac{1}{4}, z$	$4a$	$4b$ $2\times4b$	$4a$ $8c$	$4b$ $8c$	$8c$ $8c$	$2\times4a$ $2\times8c$
[2] $P4_222$ (93)		$x+\frac{1}{2}, y, z-\frac{1}{4}$	$x+\frac{1}{4}$, $y+\frac{1}{4}, z$	$2a;2b$	$2c;2d$ $2\times4i$	$2e;2f$ $4j;4m$	$4i$ $4k;4l$	$8p$ $4n;4o$	$4g;4h$ $2\times8p$
[2] $P4_2/n$ (86)			$x+\frac{1}{2}, y, z$	$4e$	$4f$ $2\times4f$	$4e$ $8g$	$2a;2b$ $8g$	$4c;4d$ $8g$	$2\times4e$ $2\times8g$
[2] $Pban$ (50)		$x+\frac{1}{2}, y, z-\frac{1}{4}$		$2a;2d$	$2b;2c$ $2\times4l$	$4k$ $4g;4j$	$4l$ $4h;4i$	$4e;4f$ $8m$	$2\times4k$ $2\times8m$
[2] $Ccce$ (68)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4}, z$	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z$	$8g$	$8h$ $2\times8h$	$4a;4b$ $16i$	$8h$ $16i$	$8c;8d$ $8e;8f$	$2\times8g$ $2\times16i$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, isomorphic									
[3] $P4_2/nbc$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a;8f$	$4b;8g$ $3\times8g$	$4c;8f$ $8h(i^*);16k$	$4d;8g$ $8i(h^*);16k$	$8e;16k$ $8j;16k$	$3\times8f$ $3\times16k$
[p] $P4_2/nbc$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$4a;\frac{p-1}{2}\times8f$	$4b;\frac{p-1}{2}\times8g$ $p\times8g$	$4c;\frac{p-1}{2}\times8f$ $8h(i^\dagger);\frac{p-1}{2}\times16k$	$4d;\frac{p-1}{2}\times8g$ $8i(h^\dagger);\frac{p-1}{2}\times16k$	$8e;\frac{p-1}{2}\times16k$ $8j;\frac{p-1}{2}\times16k$	$p\times8f$ $p\times16k$
	$p = \text{prime} > 2$; $u = 1,\ldots,p-1$								
[9] $P4_2/nbc$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$;	$\frac{1}{3}x, \frac{1}{3}y, z$;	$4a;8h;8i;16k$	$4b;8h;8i;16k$ $8g;4\times16k$	$4c;2\times8j;16k$ $3\times8h;3\times16k$	$4d;2\times16k$ $3\times8i;3\times16k$	$8e;4\times16k$ $3\times8j;3\times6k$	$8f;4\times16k$ $9\times16k$
		$\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$							
[p^2] $P4_2/nbc$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$4a;\frac{p-1}{2}\times8h$; $\frac{p-1}{2}\times8i$; $\frac{(p-1)^2}{4}\times16k$	$4b;\frac{p-1}{2}\times8h$; $\frac{p-1}{2}\times8i$; $\frac{(p-1)^2}{4}\times16k$ $8g;\frac{p^2-1}{2}\times16k$	$4c;(p-1)\times8j$; $\frac{(p-1)^2}{4}\times16k$ $p\times8h$; $\frac{p(p-1)}{2}\times16k$	$4d;\frac{p^2-1}{4}\times16k$ $p\times8i$; $\frac{p(p-1)}{2}\times16k$	$8e;\frac{p^2-1}{2}\times16k$ $p\times8j$; $\frac{p(p-1)}{2}\times16k$	$8f;\frac{p^2-1}{2}\times16k$ $p^2\times16k$
	$p = \text{prime} > 2$; $u, v = 1,\ldots,p-1$								

* origin 1

† origin 1 and $p = 4n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 134, pp. 616–617.

$P4_2/nnm$ No. 134 $P4_2/n2/n2/m$ D_{4h}^{12}

	Axes	Coordinates origin 1	Coordinates origin 2	2a	2b	4c 8i	4d 8j	4e 8k	4f 8l	4g 8m	8h 16n
I Maximal *translationengleiche* subgroups											
[2] $P\bar{4}n2$ (118)			$x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	$2a$	$2b$	$4h$ $8i$	$2c;2d$ $8i$	$4f$ $2\times4g$	$4g$ $2\times4f$	$4e$ $8i$	$2\times4h$ $2\times8i$
[2] $P\bar{4}2m$ (111)			$x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	$1a;1b$	$1c;1d$	$2e;2f$ $4i;4j$	$4m$ $4k;4l$	$4n$ $8o$	$4n$ $8o$	$2g;2h$ $2\times4n$	$2\times4m$ $2\times8o$
[2] $P4_2nm$ (102)			$x+\frac{1}{4},y-\frac{1}{4},z$	$2a$	$2a$	$4b$ $8d$	$4b$ $8d$	$4c$ $8d$	$4c$ $8d$	$2\times2a$ $2\times4c$	$2\times4b$ $2\times8d$
[2] $P4_222$ (93)		$x,y+\frac{1}{2},z$	$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$2c$	$2d$	$2a;2b$ $4l;4m$	$2e;2f$ $4j;4k$	$4o$ $2\times4n$	$4n$ $2\times4o$	$4i$ $8p$	$4g;4h$ $2\times8p$
[2] $P4_2/n$ (86)			$x,y+\frac{1}{2},z$	$2a$	$2b$	$4e$ $8g$	$4e$ $8g$	$4c$ $8g$	$4d$ $8g$	$4f$ $8g$	$2\times4e$ $2\times8g$
[2] $Pnnn$ (48)				$2a(d^*)$	$2c(b^*)$	$2b(a^*);2d(c^*)$ $4g(h^*);4i$	$4l(k^*)$ $4h(g^*);4j$	$4e$ $8m$	$4f$ $8m$	$4k(l^*)$ $8m$	$2\times4l(k^*)$ $2\times8m$
[2] $Cmme$ (67)	**a**+**b**, −**a**+**b**, **c**	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y)+\frac{1}{4},z-\frac{1}{4}$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),z$	$4g$	$4g$	$8l$ $16o$	$4a;4b$ $16o$	$4d;4e$ $8h;8k$	$4c;4f$ $8i;8j$	$2\times4g$ $8m;8n$	$2\times8l$ $2\times16o$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**											
[2] $I4_1/acd$ (142)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$8a$	$8b$	$16f$ $32g$	$16e$ $2\times16f$	$16e$ $32g$	$16c$ $2\times16e$	$16d$ $32g$	$32g$ $2\times32g$
[2] $I4_1/acd$ (142)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$8b$	$8a$	$16f$ $2\times16f$	$16e$ $32g$	$16c$ $2\times16e$	$16e$ $32g$	$16d$ $32g$	$32g$ $2\times32g$
[2] $I4_1/acd$ (142)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$8b$	$8a$	$16f$ $2\times16f$	$16e$ $32g$	$16e$ $32g$	$16c$ $2\times16e$	$16d$ $32g$	$32g$ $2\times32g$
[2] $I4_1/acd$ (142)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$8a$	$8b$	$16f$ $32g$	$16e$ $2\times16f$	$16c$ $2\times16e$	$16e$ $32g$	$16d$ $32g$	$32g$ $2\times32g$
[2] $I4_1/amd$ (141)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$4a;4b$	$8e$	$16g$ $2\times16g$	$16f$ $32i$	$16h$ $2\times16f$	$8c;8d$ $32i$	$2\times8e$ $2\times16h$	$32i$ $2\times32i$
[2] $I4_1/amd$ (141)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$8e$	$4a;4b$	$16g$ $32i$	$16f$ $2\times16g$	$8c;8d$ $32i$	$16h$ $2\times16f$	$2\times8e$ $2\times16h$	$32i$ $2\times32i$
[2] $I4_1/amd$ (141)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$8e$	$4a;4b$	$16g$ $32i$	$16f$ $2\times16g$	$16h$ $2\times16f$	$8c;8d$ $32i$	$2\times8e$ $2\times16h$	$32i$ $2\times32i$
[2] $I4_1/amd$ (141)	**a**+**b**, −**a**+**b**, 2**c**	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$\frac{1}{2}(x+y)+\frac{1}{2}$, $\frac{1}{2}(-x+y),\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$4a;4b$	$8e$	$16g$ $2\times16g$	$16f$ $32i$	$8c;8d$ $32i$	$16h$ $2\times16f$	$2\times8e$ $2\times16h$	$32i$ $2\times32i$

* origin 2

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions				
				$2a$ $4f$	$2b$ $4g$ $8k$	$4c$ $8h$ $8l$	$4d$ $8i$ $8m$	$4e$ $8j$ $16n$
Enlarged unit cell, isomorphic								
[3] $P4_2/nnm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$x, y, \frac{1}{3}z;$ $\pm(0,0,\frac{1}{3})$	$2a(b^*); 4g$ $4e(f^*); 8m$	$2b(a^*); 4g$ $3\times 4g$ $8l(k^*); 16n$	$4c; 8h$ $3\times 8h$ $8k(l^*); 16n$	$4d; 8h$ $8i(j^*); 16n$ $3\times 8m$	$4f(e^*); 8m$ $8j(i^*); 16n$ $3\times 16n$
[p] $P4_2/nnm$ $p =$ prime > 2; $u = 1,\ldots,p-1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$x, y, \frac{1}{p}z;$ $+(0,0,\frac{u}{p})$	$2a(b^\dagger); \frac{p-1}{2}\times 4g$ $4f(e^\ddagger); \frac{p-1}{2}\times 8m$	$2b(a^\dagger); \frac{p-1}{2}\times 4g$ $p\times 4g$ $8k(l^\ddagger); \frac{p-1}{2}\times 16n$	$4c; \frac{p-1}{2}\times 8h$ $p\times 8h$ $8l(k^\ddagger); \frac{p-1}{2}\times 16n$	$4d; \frac{p-1}{2}\times 8h$ $8i(j^\dagger); \frac{p-1}{2}\times 16n$ $p\times 8m$	$4e(f^\ddagger); \frac{p-1}{2}\times 8m$ $8j(i^\dagger); \frac{p-1}{2}\times 16n$ $p\times 16n$
[9] $P4_2/nnm$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z;$ $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$	$\frac{1}{3}x, \frac{1}{3}y, z;$	$2a(b^*); 8i(j^*); 8m$ $4f; 8k; 8m; 16n$	$2b(a^*); 8j(i^*); 8m$ $4g; 2\times 8m; 16n$ $3\times 8k; 3\times 16n$	$4c; 8i; 8j; 16n$ $8h; 4\times 16n$ $3\times 8l; 3\times 16n$	$4d; 8k; 8l; 16n$ $3\times 8i(j^*); 3\times 16n$ $3\times 8m; 3\times 16n$	$4e; 8l; 8m; 16n$ $3\times 8j(i^*); 3\times 16n$ $9\times 16n$
[p^2] $P4_2/nnm$ $p =$ prime > 2; $u, v = 1,\ldots,p-1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z;$ $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x, \frac{1}{p}y, z;$ $+(\frac{u}{p},\frac{v}{p},0)$	$2a(b^\dagger); \frac{p-1}{2}\times 8i(j^\dagger);$ $\frac{p-1}{2}\times 8m;$ $\frac{(p-1)(p-3)}{8}\times 16n$ $4f; \frac{p-1}{2}\times 8k;$ $\frac{p-1}{2}\times 8m;$ $\frac{(p-1)^2}{4}\times 16n$	$2b(a^\dagger); \frac{p-1}{2}\times 8j(i^\dagger);$ $\frac{p-1}{2}\times 8m;$ $\frac{(p-1)(p-3)}{8}\times 16n$ $4g; (p-1)\times 8m;$ $\frac{(p-1)^2}{4}\times 16n$ $p\times 8k; \frac{p(p-1)}{2}\times 16n$	$4c; \frac{p-1}{2}\times 8i;$ $\frac{p-1}{2}\times 8j;$ $\frac{(p-1)^2}{4}\times 16n$ $8h; \frac{p^2-1}{2}\times 16n$ $p\times 8l;$ $\frac{p(p-1)}{2}\times 16n$	$4d; \frac{p-1}{2}\times 8k;$ $\frac{p-1}{2}\times 8l;$ $\frac{(p-1)^2}{4}\times 16n$ $p\times 8i(j^\dagger);$ $\frac{p(p-1)}{2}\times 16n$ $p\times 8m;$ $\frac{p(p-1)}{2}\times 16n$	$4e; \frac{p-1}{2}\times 8l;$ $\frac{p-1}{2}\times 8m;$ $\frac{(p-1)^2}{4}\times 16n$ $p\times 8j(i^\dagger);$ $\frac{p(p-1)}{2}\times 16n$ $p^2\times 16n$

* origin 2
† origin 2 and $p = 4n-1$
‡ origin 1 and $p = 4n-1$

$P4_2/mbc$ No. 135 $P4_2/m2_1/b2/c$ D_{4h}^{13}

	Axes	Coordinates	4a	4b	4c	4d 8g	8e 8h	8f 16i

I Maximal *translationengleiche* subgroups

Subgroup	Axes	Coordinates	4a	4b	4c	4d 8g	8e 8h	8f 16i
[2] $P\bar{4}b2$ (117)		$x,y,z+\frac{1}{4}$	$4e$	$2a;2b$	$4f$	$2c;2d$ $4g;4h$	$2\times4e$ $8i$	$2\times4f$ $2\times8i$
[2] $P\bar{4}2_1c$ (114)		$x,y,z+\frac{1}{4}$	$4c$	$2a;2b$	$4d$	$4d$ $8e$	$2\times4c$ $8e$	$2\times4d$ $2\times8e$
[2] $P4_2bc$ (106)			$4a$	$4a$	$4b$	$4b$ $8c$	$2\times4a$ $8c$	$2\times4b$ $2\times8c$
[2] $P4_22_12$ (94)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$4d$	$4d$	$4c$	$2a;2b$ $4e;4f$	$2\times4d$ $8g$	$2\times4c$ $2\times8g$
[2] $P4_2/m$ (84)			$2a;2b$	$2e;2f$	$2c;2d$	$4i$ $8k$	$4g;4h$ $2\times4j$	$2\times4i$ $2\times8k$
[2] $Pbam$ (55)			$2a;2b$	$4e$	$2c;2d$	$4f$ $8i$	$2\times4e$ $4g;4h$	$2\times4f$ $2\times8i$
[2] $Cccm$ (66)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z$	$4e;4f$	$8k$	$4c;4d$	$4a;4b$ $8g;8h$	$2\times8k$ $2\times8l$	$8i;8j$ $2\times16m$

II Maximal *klassengleiche* subgroups

Enlarged unit cell, isomorphic

Subgroup	Axes	Coordinates	4a	4b	4c	4d 8g	8e 8h	8f 16i
[3] $P4_2/mbc$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$4a;8e$	$4b;8e$	$4c;8f$	$4d;8f$ $8g;16i$	$3\times8e$ $8h;16i$	$3\times8f$ $3\times16i$
[p] $P4_2/mbc$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=\text{prime}>2$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $u=1,\dots,p-1$	$4a;\frac{p-1}{2}\times8e$	$4b;\frac{p-1}{2}\times8e$	$4c;\frac{p-1}{2}\times8f$	$4d;\frac{p-1}{2}\times8f$ $8g;\frac{p-1}{2}\times16i$	$p\times8e$ $8h;\frac{p-1}{2}\times16i$	$p\times8f$ $p\times16i$
[9] $P4_2/mbc$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z;$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$	$4a;4\times8h$	$4b;2\times16i$	$4c;4\times8h$	$4d;2\times8g;16i$ $3\times8g;3\times16i$	$8e;4\times16i$ $9\times8h$	$8f;4\times16i$ $9\times16i$
[p^2] $P4_2/mbc$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=\text{prime}>2;$	$\frac{1}{p}x,\frac{1}{p}y,z;$ $+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\dots,p-1$	$4a;\frac{p^2-1}{2}\times8h$	$4b;\frac{p^2-1}{4}\times16i$	$4c;\frac{p^2-1}{2}\times8h$	$4d;(p-1)\times8g;$ $\frac{(p-1)^2}{4}\times16i$ $p\times8g;$ $\frac{p(p-1)}{2}\times16i$	$8e;\frac{p^2-1}{2}\times16i$ $p^2\times8h$	$8f;\frac{p^2-1}{2}\times16i$ $p^2\times16i$

D_{4h}^{14} $P4_2/m2_1/n2/m$ No. 136 $P4_2/mnm$

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$4c$	$4d$	$4e$	$4f$
				$4g$	$8h$	$8i$	$8j$	$16k$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}n2$ (118)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2d$	$2c$	$4e$	$2a;2b$	$4h$	$4g$
				$4f$	$2\times 4e$	$8i$	$8i$	$2\times 8i$
[2] $P\bar{4}2_1m$ (113)		$x+\frac{1}{2},y,z+\frac{1}{4}$	$2c$	$2c$	$4d$	$2a;2b$	$2\times 2c$	$4e$
				$4e$	$2\times 4d$	$8f$	$2\times 4e$	$2\times 8f$
[2] $P4_2nm$ (102)			$2a$	$2a$	$4b$	$4b$	$2\times 2a$	$4c$
				$4c$	$2\times 4b$	$8d$	$2\times 4c$	$2\times 8d$
[2] $P4_22_12$ (94)			$2a$	$2b$	$4d$	$4d$	$4c$	$4e$
				$4f$	$2\times 4d$	$8g$	$8g$	$2\times 8g$
[2] $P4_2/m$ (84)		$x+\frac{1}{2},y,z$	$2d$	$2c$	$2a;2b$	$2e;2f$	$4i$	$4j$
				$4j$	$4g;4h$	$2\times 4j$	$8k$	$2\times 8k$
[2] $Pnnm$ (58)			$2a$	$2b$	$2c;2d$	$4f$	$4e$	$4g$
				$4g$	$2\times 4f$	$2\times 4g$	$8h$	$2\times 8h$
[2] $Cmmm$ (65)	$\mathbf{a}-\mathbf{b}$,	$\frac{1}{2}(x-y)$,	$2a;2c$	$2b;2d$	$4e;4f$	$8m$	$4k;4l$	$4h;4i$
	$\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x+y),z$		$4g;4j$	$2\times 8m$	$8p;8q$	$8n;8o$	$2\times 16r$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, isomorphic								
[3] $P4_2/mnm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$;	$2a;4e$	$2b;4e$	$4c;8h$	$4d;8h$	$3\times 4e$	$4f;8j$
		$\pm(0,0,\frac{1}{3})$		$4g;8j$	$3\times 8h$	$8i;16k$	$3\times 8j$	$3\times 16k$
[p] $P4_2/mnm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$;	$2a;\frac{p-1}{2}\times 4e$	$2b;\frac{p-1}{2}\times 4e$	$4c;\frac{p-1}{2}\times 8h$	$4d;\frac{p-1}{2}\times 8h$	$p\times 4e$	$4f;\frac{p-1}{2}\times 8j$
		$+(0,0,\frac{u}{p})$		$4g;\frac{p-1}{2}\times 8j$	$p\times 8h$	$8i;\frac{p-1}{2}\times 16k$	$p\times 8j$	$p\times 16i$
	$p=$ prime >2							
		$u=1,\ldots,p-1$						
[9] $P4_2/mnm$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,z$;	$2a;4f;4g;8i$	$2b;4f;4g;8i$	$4c;4\times 8i$	$4d;2\times 16k$	$4e;2\times 8j;16k$	$3\times 4f;3\times 8i$
		$\pm(\frac{1}{3},0,0)$;		$3\times 4g;3\times 8i$	$8h;4\times 16k$	$9\times 8i$	$3\times 8j;3\times 16k$	$9\times 16k$
		$\pm(0,\frac{1}{3},0)$;						
		$\pm(\frac{1}{3},\frac{1}{3},0)$;						
		$\pm(\frac{1}{3},\frac{2}{3},0)$						
[p^2] $P4_2/mnm$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$;	$2a;\frac{p-1}{2}\times 4f$;	$2b;\frac{p-1}{2}\times 4f$	$4c;\frac{p^2-1}{2}\times 8i$	$4d;\frac{p^2-1}{4}\times 16k$	$4e;(p-1)\times 8j$;	$p\times 4f$;
		$+(\frac{u}{p},\frac{v}{p},0)$	$\frac{p-1}{2}\times 4g$;	$\frac{p-1}{2}\times 4g$;			$\frac{(p-1)^2}{4}\times 16k$	$\frac{p(p-1)}{2}\times 8i$
	$p=$ prime >2;		$\frac{(p-1)^2}{4}\times 8i$	$\frac{(p-1)^2}{4}\times 8i$				
		$u,v=1,\ldots,p-1$		$p\times 4g$;	$8h;\frac{p^2-1}{2}\times 16k$	$p^2\times 8i$	$p\times 8j$;	$p^2\times 16k$
				$\frac{p(p-1)}{2}\times 8i$			$\frac{p(p-1)}{2}\times 16k$	

$P4_2/nmc$ No. 137 $P4_2/n2_1/m2/c$ D_{4h}^{15}

	Axes	Coordinates origin 1	origin 2	Wyckoff positions 2a	2b	4c	4d	8e
						8f	8g	16h
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}m2$			$x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	$1a;1c$	$1b;1d$	$2e;2f$	$2\times2g$	$8l$
(115)						$4h;4i$	$4j;4k$	$2\times8l$
[2] $P\bar{4}2_1c$			$x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	$2a$	$2b$	$4c$	$4d$	$8e$
(114)						$8e$	$8e$	$2\times8e$
[2] $P4_2mc$		$x+\frac{1}{2},y,z$	$x+\frac{1}{4},y+\frac{1}{4},z$	$2c$	$2c$	$2\times2c$	$2a;2b$	$8f$
(105)						$8f$	$4d;4e$	$2\times8f$
[2] $P4_22_12$			$x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	$2a$	$2b$	$4c$	$4d$	$8g$
(94)						$4e;4f$	$8g$	$2\times8g$
[2] $P4_2/n$			$x,y+\frac{1}{2},z$	$2a$	$2b$	$4f$	$4e$	$4c;4d$
(86)						$8g$	$8g$	$2\times8g$
[2] $Pmmn$		$x,y,z+\frac{1}{4}$		$2a(b^*)$	$2a(b^*)$	$2\times2a(b^*)$	$2\times2b(a^*)$	$4c;4d$
(59)						$8g$	$4e;4f$	$2\times8g$
[2] $Ccce$	$\mathbf{a}+\mathbf{b}$,	$\frac{1}{2}(x+y)$,	$\frac{1}{2}(x+y)$,	$4a(b^*)$	$4b(a^*)$	$8g$	$8h$	$8c;8d$
(68)	$-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{2}(-x+y),z$	$\frac{1}{2}(-x+y),z$			$8e;8f$	$16i$	$2\times16i$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, isomorphic								
[3] $P4_2/nmc$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a(b^*);4c$	$2b(a^*);4c$	$3\times4c$	$3\times4d$	$8e;16h$
						$8f;16h$	$3\times8g$	$3\times16h$
[p] $P4_2/nmc$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a(b^\dagger);\frac{p-1}{2}\times4c$	$2b(a^\dagger);\frac{p-1}{2}\times4c$	$p\times4c$	$p\times4d$	$8e;\frac{p-1}{2}\times16h$
	$p=$ prime >2; $u=1,\ldots,p-1$					$8f;\frac{p-1}{2}\times16h$	$p\times8g$	$p\times16h$
[9] $P4_2/nmc$	$3\mathbf{a},3\mathbf{b},\mathbf{c}$	$\underbrace{\frac{1}{3}x,\frac{1}{3}y,z; \quad \frac{1}{3}x,\frac{1}{3}y,z;}$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0);\pm(\frac{1}{3},\frac{2}{3},0)$		$2a(b^*);8f;8g$	$2b(a^*);8f;8g$	$4c;2\times8g;16h$	$4d;2\times8g;16h$	$8e;4\times16h$
						$3\times8f;3\times16h$	$3\times8g;3\times16h$	$9\times16h$
[p^2] $P4_2/nmc$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a(b^\dagger);\frac{p-1}{2}\times8f$; $\frac{p-1}{2}\times8g$; $\frac{(p-1)(p-3)}{8}\times16h$	$2b(a^\dagger);\frac{p-1}{2}\times8f$; $\frac{p-1}{2}\times8g$; $\frac{(p-1)(p-3)}{8}\times16h$	$4c;(p-1)\times8g$; $\frac{(p-1)^2}{4}\times16h$	$4d;(p-1)\times8g$; $\frac{(p-1)^2}{4}\times16h$	$8e;\frac{p^2-1}{2}\times16h$
	$p=$ prime >2; $u,v=1,\ldots,p-1$					$p\times8f$; $\frac{p(p-1)}{2}\times16h$	$p\times8g$; $\frac{p(p-1)}{2}\times16h$	$p^2\times16h$

* origin 2

† origin 2 and $p=4n-1$

D_{4h}^{16} $P4_2/n2_1/c2/m$ No. 138 $P4_2/ncm$

	Axes	Coordinates: origin 1	Coordinates: origin 2	Wyckoff positions: $4a$ $8f$	$4b$ $8g$	$4c$ $8h$	$4d$ $8i$	$4e$ $16j$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{4}c2$ (116)			$x+\frac{1}{4}, y-\frac{1}{4}, z+\frac{1}{4}$	$2a;2b$ $4g;4h$	$2c;2d$ $2\times4e$	$4e$ $2\times4f$	$4f$ $8j$	$4i$ $2\times8j$
[2] $P\bar{4}2_1m$ (113)			$x+\frac{1}{4}, y-\frac{1}{4}, z+\frac{1}{4}$	$4d$ $2\times4d$	$2a;2b$ $8f$	$4e$ $8f$	$4e$ $2\times4e$	$2\times2c$ $2\times8f$
[2] $P4_2cm$ (101)		$x+\frac{1}{2}, y, z$	$x+\frac{1}{4}, y+\frac{1}{4}, z$	$4c$ $2\times4c$	$4c$ $8e$	$4d$ $8e$	$4d$ $2\times4d$	$2a;2b$ $2\times8e$
[2] $P4_22_12$ (94)		$x, y, z-\frac{1}{4}$	$x+\frac{1}{4}, y-\frac{1}{4}, z$	$2a;2b$ $2\times4c$	$4c$ $2\times4e$	$4e$ $2\times4f$	$4f$ $8g$	$4d$ $2\times8g$
[2] $P4_2/n$ (86)			$x+\frac{1}{2}, y, z$	$4f$ $2\times4f$	$2a;2b$ $8g$	$4c$ $8g$	$4d$ $8g$	$4e$ $2\times8g$
[2] $Pccn$ (56)		$x+\frac{1}{4}, y-\frac{1}{4}, z-\frac{1}{4}$		$4d$ $2\times4d$	$4d$ $8e$	$4b$ $8e$	$4a$ $8e$	$4c$ $2\times8e$
[2] $Cmme$ (67)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y)-\frac{1}{4}, \frac{1}{2}(x+y), z-\frac{1}{4}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$4a;4b$ $2\times8l$	$8l$ $8i;8j$	$4d;4e$ $8h;8k$	$4c;4f$ $8m;8n$	$2\times4g$ $2\times16o$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, isomorphic								
[3] $P4_2/ncm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$4a;8f$ $3\times8f$	$4b;8f$ $8g(h^*);16j$	$4c(d^*);8i$ $8h(g^*);16j$	$4d(c^*);8i$ $3\times8i$	$3\times4e$ $3\times16j$
[p] $P4_2/ncm$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p=$ prime >2; $u=1,\dots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$4a;\frac{p-1}{2}\times8f$ $p\times8f$	$4b;\frac{p-1}{2}\times8f$ $8g(h^\dagger);\frac{p-1}{2}\times16j$	$4c(d^\dagger);\frac{p-1}{2}\times8i$ $8h(g^\dagger);\frac{p-1}{2}\times16j$	$4d(c^\dagger);\frac{p-1}{2}\times8i$ $p\times8i$	$p\times4e$ $p\times16j$
[9] $P4_2/ncm$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\underbrace{\frac{1}{3}x, \frac{1}{3}y, z; \quad \frac{1}{3}x, \frac{1}{3}y, z;}$ $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{2}{3},0)$		$4a;8g;8h;16j$ $8f;4\times16j$	$4b;2\times16j$ $3\times8g;3\times16j$	$4c;8g;8i;16j$ $3\times8h;3\times16j$	$4d;8h;8i;16j$ $3\times8i;3\times16j$	$4e;2\times8i;16j$ $9\times16j$
[p^2] $P4_2/ncm$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p=$ prime >2; $u,v=1,\dots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$4a;\frac{p-1}{2}\times8g;$ $\frac{p-1}{2}\times8h;$ $\frac{(p-1)^2}{4}\times16j$ $8f;\frac{p^2-1}{2}\times16j$	$4b;\frac{p^2-1}{4}\times16j$ $p\times8g;$ $\frac{p(p-1)}{2}\times16j$	$4c;\frac{p-1}{2}\times8g;$ $\frac{p-1}{2}\times8i;$ $\frac{(p-1)^2}{4}\times16j$ $p\times8h;$ $\frac{p(p-1)}{2}\times16j$	$4d;\frac{p-1}{2}\times8h;$ $\frac{p-1}{2}\times8i;$ $\frac{(p-1)^2}{4}\times16j$ $p\times8i;$ $\frac{p(p-1)}{2}\times16j$	$4e;(p-1)\times8i;$ $\frac{(p-1)^2}{4}\times16j$ $p^2\times16j$

* origin 1

† origin 1 and $p=4n-1$

*I*4/*mmm* No. 139 *I*4/*m*2/*m*2/*m* D_{4h}^{17}

	Axes	Coordinates	Wyckoff positions										
			2*a*	2*b*	4*c*	4*d*	4*e*	8*f*	8*g*	8*h*	8*i*	8*j* 16*m*	16*k* 16*n*	16*l* 32*o*

I Maximal *translationengleiche* subgroups

Subgroup	Axes	Coordinates	2*a*	2*b*	4*c*	4*d*	4*e*	8*f*	8*g*	8*h*	8*i*	8*j* 16*m*	16*k* 16*n*	16*l* 32*o*
[2] $I\bar{4}2m$ (121)			2*a*	2*b*	4*c*	4*d*	4*e*	8*i*	8*h*	8*i*	8*f*	8*g* 2×8*i*	16*j* 16*j*	16*j* 2×16*j*
[2] $I\bar{4}m2$ (119)			2*a*	2*b*	4*f*	2*c*; 2*d*	4*e*	8*h*	2×4*f*	8*g*	8*i*	8*i* 16*j*	2×8*h* 2×8*i*	16*j* 2×16*j*
[2] *I*4*mm* (107)			2*a*	2*a*	4*b*	4*b*	2×2*a*	8*c*	2×4*b*	8*c*	8*d*	8*d* 2×8*c*	16*e* 2×8*d*	16*e* 2×16*e*
[2] *I*422 (97)			2*a*	2*b*	4*c*	4*d*	4*e*	8*j*	8*f*	8*g*	8*h*	8*i* 16*k*	2×8*j* 16*k*	16*k* 2×16*k*
[2] *I*4/*m* (87)			2*a*	2*b*	4*c*	4*d*	4*e*	8*f*	8*g*	8*h*	8*h*	8*h* 16*i*	16*i* 16*i*	2×8*h* 2×16*i*
[2] *Immm* (71)			2*a*	2*c*	2*b*; 2*d*	4*j*	4*i*	8*k*	2×4*j*	8*n*	4*e*; 4*g*	4*f*; 4*h* 16*o*	16*o* 8*l*; 8*m*	2×8*n* 2×16*o*
[2] *Fmmm* (69)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)$, $\frac{1}{2}(x+y), z$	4*a*	4*b*	8*e*	8*f*	8*i*	8*c*; 8*d*	16*j*	8*g*; 8*h*	16*o*	16*o* 16*m*; 16*n*	16*k*; 16*l* 32*p*	2×16*o* 2×32*p*

II Maximal *klassengleiche* subgroups

Loss of centring translations

Subgroup	Coordinates	2*a*	2*b*	4*c*	4*d*	4*e*	8*f*	8*g*	8*h*	8*i*	8*j* 16*m*	16*k* 16*n*	16*l* 32*o*
[2] $P4_2/nmc$ (137)	origin 1: x, y, z origin 2: $x+\frac{1}{4}, y-\frac{1}{4}, z+\frac{1}{4}$	2*a*	2*b*	4*d*	4*d*	4*c*	8*e*	2×4*d*	8*f*	8*g*	8*g* 16*h*	16*h* 2×8*g*	16*h* 2×16*h*
[2] $P4_2/mnm$ (136)		2*a*	2*b*	4*c*	4*d*	4*e*	8*j*	8*h*	4*f*; 4*g*	8*i*	8*i* 2×8*j*	16*k* 16*k*	2×8*i* 2×16*k*
[2] $P4_2/nnm$ (134)	origin 1: x, y, z origin 2: $x+\frac{1}{4}, y-\frac{1}{4}, z+\frac{1}{4}$	2*a*	2*b*	4*c*	4*d*	4*g*	4*e*; 4*f*	8*h*	8*m*	8*i*	8*j* 2×8*m*	8*k*; 8*l* 16*n*	16*n* 2×16*n*
[2] $P4_2/mmc$ (131)	$x+\frac{1}{2}, y, z$	2*d*	2*c*	2*a*; 2*b*	2*e*; 2*f*	4*i*	8*n*	4*g*; 4*h*	8*q*	4*j*; 4*k*	4*l*; 4*m* 16*r*	2×8*n* 8*o*; 8*p*	2×8*q* 2×16*r*
[2] $P4/nmm$ (129)	origin 1: $x, y+\frac{1}{2}, z+\frac{1}{4}$ origin 2: $x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	2*c*	2*c*	4*f*	2*a*; 2*b*	2×2*c*	4*d*; 4*e*	2×4*f*	8*j*	8*i*	8*i* 2×8*j*	8*g*; 8*h* 2×8*i*	16*k* 2×16*k*
[2] $P4/mnc$ (128)		2*a*	2*b*	4*c*	4*d*	4*e*	8*g*	8*f*	8*h*	8*h*	8*h* 16*i*	2×8*g* 16*i*	2×8*h* 2×16*i*
[2] $P4/nnc$ (126)	origin 1: x, y, z origin 2: $x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	2*a*	2*b*	4*c*	4*d*	4*e*	8*f*	8*g*	8*h*	8*i*	8*j* 16*k*	16*k* 16*k*	16*k* 2×16*k*
[2] $P4/mmm$ (123)		1*a*; 1*d*	1*b*; 1*c*	2*e*; 2*f*	4*i*	2*g*; 2*h*	8*r*	2×4*i*	4*j*; 4*k*	4*l*; 4*o*	4*m*; 4*n* 2×8*r*	16*u* 8*s*; 8*t*	8*p*; 8*q* 2×16*u*

	Axes	Coordinates	Wyckoff positions $2a$	$2b$ $8g$	$4c$ $8h$ $16l$	$4d$ $8i$ $16m$	$4e$ $8j$ $16n$	$8f$ $16k$ $32o$
Enlarged unit cell, isomorphic								
[3] $I4/mmm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$	$2b$; $4e$ $3\times8g$	$4c$; $8g$ $8h$; $16m$ $16l$; $32o$	$4d$; $8g$ $8i$; $16n$ $3\times16m$	$3\times4e$ $8j$; $16n$ $3\times16n$	$8f$; $16m$ $16k$; $32o$ $3\times32o$
[p] $I4/mmm$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p = \text{prime} > 2$; $u = 1,\dots,p-1$	$2a$; $\frac{p-1}{2}\times4e$	$2b$; $\frac{p-1}{2}\times4e$ $p\times8g$	$4c$; $\frac{p-1}{2}\times8g$ $8h$; $\frac{p-1}{2}\times16m$ $16l$; $\frac{p-1}{2}\times32o$	$4d$; $\frac{p-1}{2}\times8g$ $8i$; $\frac{p-1}{2}\times16n$ $p\times16m$	$p\times4e$ $8j$; $\frac{p-1}{2}\times16n$ $p\times16n$	$8f$; $\frac{p-1}{2}\times16m$ $16k$; $\frac{p-1}{2}\times32o$ $p\times32o$
[9] $I4/mmm$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a$; $8h$; $8i$	$2b$; $8h$; $8j$ $8g$; $2\times16n$; $32o$	$4c$; $8i$; $8j$; $16l$ $3\times8h$; $3\times16l$ $9\times16l$	$4d$; $16k$; $16n$ $3\times8i$; $3\times16l$ $3\times16m$; $3\times32o$	$4e$; $16m$; $16n$ $3\times8j$; $3\times16l$ $3\times16n$; $3\times32o$	$8f$; $16k$; $16m$; $32o$ $3\times16k$; $3\times32o$ $9\times32o$
[p^2] $I4/mmm$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ $p = \text{prime} > 2$; $u, v = 1,\dots,p-1$	$2a$; $\frac{p-1}{2}\times8h$; $\frac{p-1}{2}\times8i$; $\frac{(p-1)(p-3)}{8}\times16l$	$2b$; $\frac{p-1}{2}\times8h$; $\frac{p-1}{2}\times8j$; $\frac{(p-1)(p-3)}{8}\times16l$ $8g$; $(p-1)\times16n$; $\frac{(p-1)^2}{4}\times32o$	$4c$; $\frac{p-1}{2}\times8i$; $\frac{p-1}{2}\times8j$; $\frac{(p-1)^2}{4}\times16l$ $p\times8h$; $\frac{p(p-1)}{2}\times16l$ $p^2\times16l$	$4d$; $\frac{p-1}{2}\times16k$; $\frac{p-1}{2}\times16n$; $\frac{(p-1)(p-3)}{8}\times32o$ $p\times8i$; $\frac{p(p-1)}{2}\times16l$ $p\times16m$; $\frac{p(p-1)}{2}\times32o$	$4e$; $\frac{p-1}{2}\times16m$; $\frac{p-1}{2}\times16n$; $\frac{(p-1)(p-3)}{8}\times32o$ $p\times8j$; $\frac{p(p-1)}{2}\times16l$ $p\times16n$ $\frac{p(p-1)}{2}\times32o$	$8f$; $\frac{p-1}{2}\times16k$; $\frac{p-1}{2}\times16m$; $\frac{(p-1)^2}{4}\times32o$ $p\times16k$; $\frac{p(p-1)}{2}\times32o$ $p^2\times32o$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 140, pp. 624–625.

$I4/mcm$ No. 140 $I4/m2/c2/m$ D_{4h}^{18}

	Axes	Coordinates	Wyckoff positions 4a	4b	4c	4d	8e	8f	8g	8h	16i	16j	16k	16l 32m
I Maximal *translationengleiche* subgroups														
[2] $I\bar{4}2m$ (121)		$x+\frac{1}{2},y,z+\frac{1}{4}$	4c	2a; 2b	4d	4e	8i	8h	2×4e	8i	16j	8f; 8g	16j	2×8i 2×16j
[2] $I\bar{4}c2$ (120)			4a	4c	4b	4d	8e	8f	8g	8h	2×8e	16i	16i	16i 2×16i
[2] $I4cm$ (108)			4a	4b	4a	4b	8c	2×4a	2×4b	8c	16d	16d	16d	2×8c 2×16d
[2] $I422$ (97)		$x,y,z+\frac{1}{4}$	2a; 2b	4c	4e	4d	8g	2×4e	8f	8j	2×8g	8h; 8i	16k	16k 2×16k
[2] $I4/m$ (87)			4e	4d	2a; 2b	4c	8f	2×4e	8g	8h	16i	16i	2×8h	16i 2×16i
[2] $Ibam$ (72)			4a	4b	4c	4d	8e	8h	8i	8j	16k	8f; 8g	2×8j	16k 2×16k
[2] $Fmmm$ (69)	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y)+\frac{1}{4}$, $\frac{1}{2}(x+y)+\frac{1}{4},z$	8f	8i	8e	4a; 4b	8c; 8d	16j	2×8i	8g; 8h	16k; 16l	32p	2×16o	16m; 16n 2×32p
II Maximal *klassengleiche* subgroups **Loss of centring translations**														
[2] $P4_2/ncm$ (138)		origin 1: x,y,z origin 2: $x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	4a	4e	4b	4e	4c; 4d	8f	2×4e	8i	8g; 8h	16j	16j	2×8i 2×16j
[2] $P4_2/mbc$ (135)		$x+\frac{1}{2},y,z$	4d	4b	4c	4a	8g	8f	8e	8h	2×8g	16i	2×8h	16i 2×16i
[2] $P4_2/nbc$ (133)		origin 1: x,y,z origin 2: $x+\frac{1}{4},y-\frac{1}{4},z+\frac{1}{4}$	4b	4a	4d	4c	8e	8g	8f	8j	16k	8h; 8i	16k	16k 2×16k
[2] $P4_2/mcm$ (132)		$x+\frac{1}{2},y,z$	4e	2b; 2d	4f	2a; 2c	8o	8k	4g; 4h	4i; 4j	16p	8l; 8m	2×8n	2×8o 2×16p
[2] $P4/ncc$ (130)		origin 1: $x+\frac{1}{2},y,z+\frac{1}{4}$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	4c	4b	4c	4a	8d	2×4c	8e	8f	16g	16g	16g	16g 2×16g
[2] $P4/mbm$ (127)			4e	4f	2a; 2b	2c; 2d	8k	2×4e	2×4f	4g; 4h	16l	16l	8i; 8j	2×8k 2×16l
[2] $P4/nbm$ (125)		origin 1: $x,y,z+\frac{1}{4}$ origin 2: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	2a; 2b	2c; 2d	4g	4h	4e; 4f	2×4g	2×4h	8m	8i; 8j	8k; 8l	16n	2×8m 2×16n
[2] $P4/mcc$ (124)			2a; 2c	4f	2b; 2d	4e	8j	4g; 4h	8i	8m	2×8j	8k; 8l	2×8m	16n 2×16n

	Axes	Coordinates	Wyckoff positions					
			$4a$	$4b$	$4c$ $8g$	$4d$ $8h$ $16k$	$8e$ $16i$ $16l$	$8f$ $16j$ $32m$
Enlarged unit cell, isomorphic								
[3] $I4/mcm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a$; $8f$	$4b$; $8g$	$4c$; $8f$ $3\times 8g$	$4d$; $8g$ $8h$; $16l$ $16k$; $32m$	$8e$; $16l$ $16i$; $32m$ $3\times 16l$	$3\times 8f$ $16j$; $32m$ $3\times 32m$
[p] $I4/mcm$ p = prime > 2; $u = 1,\ldots,p-1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$4a$; $\frac{p-1}{2}\times 8f$	$4b$; $\frac{p-1}{2}\times 8g$	$4c$; $\frac{p-1}{2}\times 8f$ $p\times 8g$	$4d$; $\frac{p-1}{2}\times 8g$ $8h$; $\frac{p-1}{2}\times 16l$ $16k$; $\frac{p-1}{2}\times 32m$	$8e$; $\frac{p-1}{2}\times 16l$ $16i$; $\frac{p-1}{2}\times 32m$ $p\times 16l$	$p\times 8f$ $16j$; $\frac{p-1}{2}\times 32m$ $p\times 32m$
[9] $I4/mcm$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$4a$; $16i$; $16j$	$4b$; $16j$; $16l$	$4c$; $2\times 16k$ $8g$; $2\times 16l$; $32m$	$4d$; $2\times 8h$; $16k$ $3\times 8h$; $3\times 16k$ $9\times 16k$	$8e$; $16i$; $16l$; $32m$ $3\times 16i$; $3\times 32m$ $3\times 16l$; $3\times 32m$	$8f$; $2\times 32m$ $3\times 16j$; $3\times 32m$ $9\times 32m$
[p^2] $I4/mcm$ p = prime > 2; $u, v = 1,\ldots,p-1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$4a$; $\frac{p-1}{2}\times 16i$; $\frac{p-1}{2}\times 16j$; $\frac{(p-1)(p-3)}{8}\times 32m$	$4b$; $\frac{p-1}{2}\times 16j$; $\frac{p-1}{2}\times 16l$; $\frac{(p-1)(p-3)}{8}\times 32m$	$4c$; $\frac{p^2-1}{4}\times 16k$ $8g$; $(p-1)\times 16l$; $\frac{(p-1)^2}{4}\times 32m$	$4d$; $(p-1)\times 8h$; $\frac{(p-1)^2}{4}\times 16k$ $p\times 8h$; $\frac{p(p-1)}{2}\times 16k$ $p^2\times 16k$	$8e$; $\frac{p-1}{2}\times 16i$; $\frac{p-1}{2}\times 16l$; $\frac{(p-1)^2}{4}\times 32m$ $p\times 16i$; $\frac{p(p-1)}{2}\times 32m$ $p\times 16l$; $\frac{p(p-1)}{2}\times 32m$	$8f$; $\frac{p^2-1}{4}\times 32m$ $p\times 16j$; $\frac{p(p-1)}{2}\times 32m$ $p^2\times 32m$

$I4_1/amd$ No. 141 $I4_1/a2/m2/d$ D_{4h}^{19}

	Axes	Coordinates origin 1	origin 2	Wyckoff positions $4a$	$4b$ $16f$	$8c$ $16g$	$8d$ $16h$	$8e$ $32i$
I Maximal *translationengleiche* subgroups								
[2] $I\bar{4}2d$ (122)			$x, y-\frac{1}{4}, z+\frac{1}{8}$	$4a$	$4b$ $2\times8d$	$8d$ $16e$	$8d$ $16e$	$8c$ $2\times16e$
[2] $I\bar{4}m2$ (119)			$x, y-\frac{1}{4}, z+\frac{1}{8}$	$2a$; $2c$	$2b$; $2d$ $16j$	$8i$ $8g$; $8h$	$8i$ $2\times8i$	$4e$; $4f$ $2\times16j$
[2] $I4_1md$ (109)			$x, y-\frac{1}{4}, z$	$4a$	$4a$ $16c$	$8b$ $16c$	$8b$ $2\times8b$	$2\times4a$ $2\times16c$
[2] $I4_122$ (98)			$x, y-\frac{1}{4}, z+\frac{1}{8}$	$4a$	$4b$ $2\times8f$	$8f$ $8d$; $8e$	$8f$ $16g$	$8c$ $2\times16g$
[2] $I4_1/a$ (88)			$x, y+\frac{1}{2}, z$	$4a$	$4b$ $16f$	$8c$ $16f$	$8d$ $16f$	$8e$ $2\times16f$
[2] $Imma$ (74)		$x, y+\frac{1}{4}, z-\frac{1}{8}$		$4e$	$4e$ $8f$; $8g$	$4a$; $4d$ $16j$	$4b$; $4c$ $8h$; $8i$	$2\times4e$ $2\times16j$
[2] $Fddd$ (70)	$\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y), z$	$\frac{1}{2}(x+y)+\frac{1}{4}$, $\frac{1}{2}(-x+y)+\frac{1}{4}, z$	$8a$	$8b$ $32h$	$16c$ $16e$; $16f$	$16d$ $32h$	$16g$ $2\times32h$
Enlarged unit cell, isomorphic								
[3] $I4_1/amd$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x+\frac{1}{2}, y, \frac{1}{3}z-\frac{1}{4}$; $\pm(0,0,\frac{1}{3})$	$x+\frac{1}{2}, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$4a$; $8e$	$4b$; $8e$ $16f$; $32i$	$8d$; $16h$ $16g$; $32i$	$8c$; $16h$ $3\times16h$	$3\times8e$ $3\times32i$
[p] $I4_1/amd$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime; $= 4n+1$ $u = 0,\dots,p-1$	$4a(b^*)$; $\frac{p-1}{2}\times8e$	$4b(a^*)$; $\frac{p-1}{2}\times8e$ $16f$; $\frac{p-1}{2}\times32i$	$8c(d^\dagger)$; $\frac{p-1}{2}\times16h$ $16g$; $\frac{p-1}{2}\times32i$	$8d(c^\dagger)$; $\frac{p-1}{2}\times16h$ $p\times16h$	$p\times8e$ $p\times32i$
[p] $I4_1/amd$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x+\frac{1}{2}, y, \frac{1}{p}z-\frac{1}{4}$; $+(0,0,\frac{u}{p})$	$x, y+\frac{1}{2}, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime $= 4n-1$; $u = 0,\dots,p-1$	$4a(b^\ddagger)$; $\frac{p-1}{2}\times8e$	$4b(a^\ddagger)$; $\frac{p-1}{2}\times8e$ $16f$; $\frac{p-1}{2}\times32i$	$8c(d^\S)$; $\frac{p-1}{2}\times16h$ $16g$; $\frac{p-1}{2}\times32i$	$8d(c^\S)$; $\frac{p-1}{2}\times16h$ $p\times16h$	$p\times8e$ $p\times32i$
[9] $I4_1/amd$	$3\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$\underbrace{\frac{1}{3}x, \frac{1}{3}y, z;}$	$\underbrace{\frac{1}{3}x, \frac{1}{3}y+\frac{1}{2}, z;}$ $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$4a$; $16g$; $16h$	$4b$; $16g$; $16h$ $3\times16f$; $3\times32i$	$8c$; $16f$; $16h$; $32i$ $3\times16g$; $3\times32i$	$8d$; $16f$; $16h$; $32i$ $3\times16h$; $3\times32i$	$8e$; $2\times16h$; $32i$ $9\times32i$
[p^2] $I4_1/amd$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x, \frac{1}{p}y+s, z$; $+(\frac{u}{p},\frac{v}{p},0)$ p = prime > 2; $u, v = 1,\dots,p-1$ $s = 0$ if $p = 4n+1$; $s = \frac{1}{2}$ if $p = 4n-1$	$4a$; $\frac{p-1}{2}\times16g$; $\frac{p-1}{2}\times16h$; $\frac{(p-1)(p-3)}{8}\times32i$	$4b$; $\frac{p-1}{2}\times16g$; $\frac{p-1}{2}\times16h$; $\frac{(p-1)(p-3)}{8}\times32i$ $p\times16f$; $\frac{p(p-1)}{2}\times32i$	$8c$; $\frac{p-1}{2}\times16f$; $\frac{p-1}{2}\times16h$; $\frac{(p-1)^2}{4}\times32i$ $p\times16g$; $\frac{p(p-1)}{2}\times32i$	$8d$; $\frac{p-1}{2}\times16f$; $\frac{p-1}{2}\times16h$; $\frac{(p-1)^2}{4}\times32i$ $p\times16h$; $\frac{p(p-1)}{2}\times32i$	$8e$; $(p-1)\times16h$; $\frac{(p-1)^2}{4}\times32i$ $p^2\times32i$

* origin 2 and $p = 8n+5$ † origin 1 and $p = 8n+5$
‡ origin 2 and $p = 8n+3$ § origin 1 and $p = 8n+3$

D_{4h}^{20} $I4_1/a2/c2/d$ No. 142 $I4_1/acd$

	Axes	Coordinates		Wyckoff positions			
		origin 1	origin 2	$8a$	$8b$ $16e$	$16c$ $16f$	$16d$ $32g$
I Maximal *translationengleiche* subgroups							
[2] $I\bar{4}2d$ (122)	(or: **b**, −**a**, **c**	$x,y+\frac{1}{2},z+\frac{1}{4}$ $y,-x,z$	$x,y+\frac{1}{4},z+\frac{3}{8}$ $y-\frac{1}{4},-x,z+\frac{1}{8}$)	$4a;4b$	$8c$ $2\times8d$	$16e$ $16e$	$2\times8c$ $2\times16e$
[2] $I\bar{4}c2$ (120)			$x,y-\frac{1}{4},z+\frac{1}{8}$	$4b;4c$	$4a;4d$ $16i$	$16i$ $8e;8h$	$8f;8g$ $2\times16i$
[2] $I4_1cd$ (110)			$x,y-\frac{1}{4},z+\frac{1}{8}$	$8a$	$8a$ $16b$	$16b$ $16b$	$2\times8a$ $2\times16b$
[2] $I4_122$ (98)		$x,y,z+\frac{1}{4}$	$x,y-\frac{1}{4},z+\frac{3}{8}$	$8c$	$4a;4b$ $2\times8f$	$16g$ $8d;8e$	$2\times8c$ $2\times16g$
[2] $I4_1/a$ (88)			$x,y+\frac{1}{2},z$	$4a;4b$	$8e$ $16f$	$8c;8d$ $16f$	$2\times8e$ $2\times16f$
[2] $Ibca$ (73)		$x,y+\frac{1}{4},z-\frac{1}{8}$		$8e$	$8e$ $8c;8d$	$8a;8b$ $16f$	$2\times8e$ $2\times16f$
[2] $Fddd$ (70)	**a**+**b**, −**a**+**b**, **c**	$\frac{1}{2}(x+y)+\frac{1}{4}$, $\frac{1}{2}(-x+y)+\frac{1}{4},z$	$\frac{1}{2}(x+y)$, $\frac{1}{2}(-x+y),z$	$16g$	$8a;8b$ $32h$	$16c;16d$ $16e;16f$	$2\times16g$ $2\times32h$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**							
[3] $I4_1/acd$	**a**, **b**, 3**c**	$x+\frac{1}{2},y,\frac{1}{3}z+\frac{1}{4}$; $\pm(0,0,\frac{1}{3})$	$x+\frac{1}{2},y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$8a;16d$	$8b;16d$ $16e;32g$	$16c;32g$ $16f;32g$	$3\times16d$ $3\times32g$
[p] $I4_1/acd$	**a**, **b**, p**c**	$x+s,y,\frac{1}{p}z+\frac{1}{2}s$; $+(0,0,\frac{u}{p})$	$x+s,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$8a;\frac{p-1}{2}\times16d$	$8b;\frac{p-1}{2}\times16d$ $16e;\frac{p-1}{2}\times32g$	$16c;\frac{p-1}{2}\times32g$ $16f;\frac{p-1}{2}\times32g$	$p\times16d$ $p\times32g$
	$p=$ prime >2; $u=0,\ldots,p-1$ $s=0$ if $p=4n+1$; $s=\frac{1}{2}$ if $p=4n-1$						
[9] $I4_1/acd$	3**a**, 3**b**, **c**	$\frac{1}{3}x,\frac{1}{3}y,z$;	$\frac{1}{3}x,\frac{1}{3}y+\frac{1}{2},z$;	$8a;2\times32g$	$8b;2\times16f;32g$ $3\times16e;3\times32g$	$16c;4\times32g$ $3\times16f;3\times32g$	$16d;4\times32g$ $9\times32g$
		$\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{2}{3},0)$					
[p^2] $I4_1/acd$	p**a**,p**b**,**c**	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$\frac{1}{p}x,\frac{1}{p}y+s,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$8a;\frac{p^2-1}{4}\times32g$	$8b;(p-1)\times16f$; $\frac{(p-1)^2}{4}\times32g$ $p\times16e$; $\frac{p(p-1)}{2}\times32g$	$16c;\frac{p^2-1}{2}\times32g$ $p\times16f$; $\frac{p(p-1)}{2}\times32g$	$16d;\frac{p^2-1}{2}\times32g$ $p^2\times32g$
	$p=$ prime >2; $u,v=1,\ldots,p-1$ $s=0$ if $p=4n+1$; $s=\frac{1}{2}$ if $p=4n-1$						

$P3$ No. 143 C_3^1

	Axes	Coordinates	Wyckoff positions 1a	1b	1c	3d
I Maximal *translationengleiche* subgroups						
[3] $P1$ (1)			1a	1a	1a	3×1a
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[3] $P3_2$ (145)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3a	3a	3a	3×3a
[3] $P3_1$ (144)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3a	3a	3a	3×3a
[3] $R3$ (146)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3×3a	9b	9b	3×9b
[3] $R3$ (146)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	9b	3×3a	9b	3×9b
[3] $R3$ (146)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	9b	9b	3×3a	3×9b
[3] $R3$ (146)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3×3a	9b	9b	3×9b
[3] $R3$ (146)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	9b	3×3a	9b	3×9b
[3] $R3$ (146)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	9b	9b	3×3a	3×9b
Enlarged unit cell, isomorphic						
[2] $P3$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2×1a	2×1b	2×1c	2×3d
[3] $P3$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3×1a	3×1b	3×1c	3×3d
[p] $P3$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$; $p = \text{prime}; u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	p×1a	p×1b	p×1c	p×1d
[3] $P3$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3},\frac{2}{3},0)$	1a; 1b; 1c	3d	3d	3×3d
[3] $P3$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3},\frac{2}{3},0)$	3d	1a; 1b; 1c	3d	3×3d
[3] $P3$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3},\frac{2}{3},0)$	3d	3d	1a; 1b; 1c	3×3d
[7] $P3$	$3\mathbf{a}+\mathbf{b}, -\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z; \pm(\frac{1}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{2}{7},0); \pm(\frac{5}{7},\frac{1}{7},0)$	1a; 2×3d	1b; 2×3d	1c; 2×3d	7×3d
[7] $P3$	$3\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z; \pm(\frac{2}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{1}{7},0); \pm(\frac{1}{7},\frac{5}{7},0)$	1a; 2×3d	1c; 2×3d	1b; 2×3d	7×3d
[p] $P3$	$q\mathbf{a}+r\mathbf{b}, -r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$; $p = \text{prime} = q^2-qr+r^2 = 6n+1$; $q, r = 1,2,\ldots;\ q > r;\ u = 1,\ldots,p-1$	$\frac{1}{p}((q-r)x+ry), \frac{1}{p}(-rx+qy), z; +(\frac{ur}{p},\frac{uq}{p},0)$	1a; $\frac{p-1}{3}$×3d	1b(c*); $\frac{p-1}{3}$×3d	1c(b*); $\frac{p-1}{3}$×3d	p×3d
[4] $P3$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	1a; 3d	1c; 3d	1b; 3d	4×3d
[p^2] $P3$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$; $p = \text{prime} = 3n-1;\ u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	1a; $\frac{p^2-1}{3}$×3d	1c; $\frac{p^2-1}{3}$×3d	1b; $\frac{p^2-1}{3}$×3d	p^2×3d

* $q+r = 3n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 144, p. 629.

$P3_1$ No. 144 C_3^2 | C_3^3 No. 145 $P3_2$

	Axes	Coordinates	Wyckoff Positions		Axes	Coordinates
			$3a$			
I Maximal *translationengleiche* subgroups						
[3] $P1$ (1)			$3{\times}1a$	[3] $P1$ (1)		
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[2] $P3_2$ (145)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2{\times}3a$	[2] $P3_1$ (144)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$
[p] $P3_2$ (145)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p = \text{prime} = 3n-1;\ u = 1,\ldots,p-1$	$p{\times}3a$	[p] $P3_1$ (144)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p = \text{prime} = 3n-1;\ u = 1,\ldots,p-1$
[7] $P3_1$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z;\ \pm(0,0,\frac{1}{7});$ $\pm(0,0,\frac{2}{7});\ \pm(0,0,\frac{3}{7})$	$7{\times}3a$	[7] $P3_2$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z;\ \pm(0,0,\frac{1}{7});$ $\pm(0,0,\frac{2}{7});\ \pm(0,0,\frac{3}{7})$
[p] $P3_1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p = \text{prime} = 6n+1;\ u = 1,\ldots,p-1$	$p{\times}3a$	[p] $P3_2$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p = \text{prime} = 6n+1;\ u = 1,\ldots,p-1$
[3] $P3_1$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$3{\times}3a$	[3] $P3_2$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$
[3] $P3_1$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$3{\times}3a$	[3] $P3_2$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$
[3] $P3_1$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$3{\times}3a$	[3] $P3_2$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$
[7] $P3_1$	$3\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z;$ $\pm(\frac{1}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{2}{7},0);\ \pm(\frac{5}{7},\frac{1}{7},0)$	$7{\times}3a$	[7] $P3_2$	$3\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z;$ $\pm(\frac{1}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{2}{7},0);\ \pm(\frac{5}{7},\frac{1}{7},0)$
[7] $P3_1$	$3\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z;$ $\pm(\frac{2}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{1}{7},0);\ \pm(\frac{1}{7},\frac{5}{7},0)$	$7{\times}3a$	[7] $P3_2$	$3\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z;$ $\pm(\frac{2}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{1}{7},0);\ \pm(\frac{1}{7},\frac{5}{7},0)$
[p] $P3_1$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$	$\frac{1}{p}((q-r)x+ry)$, $\frac{1}{p}(-rx+qy), z;\ +(\frac{ur}{p},\frac{uq}{p},0)$ $p = \text{prime} = q^2-qr+r^2 = 6n+1;$ $q, r = 1,2,\ldots;\ q > r;\ u = 1,\ldots,p-1$	$p{\times}3a$	[p] $P3_2$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$	$\frac{1}{p}((q-r)x+ry)$, $\frac{1}{p}(-rx+qy), z;\ +(\frac{ur}{p},\frac{uq}{p},0)$ $p = \text{prime} = q^2-qr+r^2 = 6n+1;$ $q, r = 1,2,\ldots;\ q > r;\ u = 1,\ldots,p-1$
[4] $P3_1$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z;\ +(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);\ +(\frac{1}{2},\frac{1}{2},0)$	$4{\times}3a$	[4] $P3_2$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z;\ +(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);\ +(\frac{1}{2},\frac{1}{2},0)$
[p^2] $P3_1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$ $p = \text{prime} = 3n-1;\ u, v = 1,\ldots,p-1$	$p^2{\times}3a$	[p^2] $P3_2$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$ $p = \text{prime} = 3n-1;\ u, v = 1,\ldots,p-1$

$R3$ No. 146 C_3^4

HEXAGONAL AXES

	Axes	Coordinates	Wyckoff positions $3a$	$9b$
I Maximal *translationengleiche* subgroups				
[3] $P1$ (1)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	$x+z, -x+y+z, -y+z$	$1a$	$3\times1a$
	rhombohedral axes: $\mathbf{a}, \mathbf{b}, \mathbf{c}$	x, y, z		
II Maximal *klassengleiche* subgroups				
Loss of centring translations				
[3] $P3_2$ (145)		$x-\frac{1}{3}, y, z$	$3a$	$3\times3a$
[3] $P3_1$ (144)		$x+\frac{1}{3}, y, z$	$3a$	$3\times3a$
[3] $P3$ (143)			$1a; 1b; 1c$	$3\times3d$
Enlarged unit cell, isomorphic				
[2] $R3$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2\times3a$	$2\times9b$
[p] $R3$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$ $p = \text{prime} = 3n-1$; $u = 1,\ldots,p-1$	$-x, -y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times3a$	$p\times9b$
[p] $R3$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} = 6n+1$; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times3a$	$p\times9b$
[7] $R3$	$3\mathbf{a}+\mathbf{b}, -\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z$; $\pm(\frac{1}{7},\frac{3}{7},0)$; $\pm(\frac{5}{7},\frac{1}{7},0)$; $\pm(\frac{3}{7},\frac{2}{7},0)$	$3a; 2\times9b$	$7\times9b$
[7] $R3$	$\mathbf{a}+3\mathbf{b}, -3\mathbf{a}-2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(-2x+3y), \frac{1}{7}(-3x+y), z$; $\pm(\frac{3}{7},\frac{1}{7},0)$; $\pm(\frac{1}{7},\frac{5}{7},0)$; $\pm(\frac{2}{7},\frac{3}{7},0)$	$3a; 2\times9b$	$7\times9b$
[p] $R3$	$q\mathbf{a}+r\mathbf{b}, -r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$ $p = q^2-qr+r^2 = \text{prime} = 6n+1$; $q, r = 1,2,\ldots$; $q \neq r$; $q+r = 3n+1$; $u = 1,\ldots,p-1$	$\frac{1}{p}((q-r)x+ry), \frac{1}{p}(-rx+qy), z$; $+(\frac{ur}{p},\frac{uq}{p},0)$	$3a; \frac{1}{3}(p-1)\times9b$	$p\times9b$
[4] $R3$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$3a; 9b$	$4\times9b$
[p^2] $R3$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$ $p = \text{prime} = 3n-1$; $u, v = 1,\ldots,p-1$	$-\frac{1}{p}x, -\frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$3a; \frac{1}{3}(p^2-1)\times9b$	$p^2\times9b$

C_{3i}^1 No. 147 $P\bar{3}$

	Axes	Coordinates	1*a*	1*b*	2*c*	2*d*	3*e*	3*f*	6*g*
I Maximal *translationengleiche* subgroups									
[2] $P3$ (143)			$1a$	$1a$	$2\times1a$	$1b;1c$	$3d$	$3d$	$2\times3d$
[3] $P\bar{1}$ (2)			$1a$	$1b$	$2i$	$2i$	$1c;1d;1e$	$1f;1g;1h$	$3\times2i$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[3] $R\bar{3}$ (148)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3a;6c$	$3b;6c$	$3\times6c$	$18f$	$9e;18f$	$9d;18f$	$3\times18f$
[3] $R\bar{3}$ (148)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3a;6c$	$3b;6c$	$3\times6c$	$18f$	$9e;18f$	$9d;18f$	$3\times18f$
Enlarged unit cell, isomorphic									
[2] $P\bar{3}$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a;1b$	$2c$	$2\times2c$	$2\times2d$	$3e;3f$	$6g$	$2\times6g$
[2] $P\bar{3}$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2c$	$1a;1b$	$2\times2c$	$2\times2d$	$6g$	$3e;3f$	$2\times6g$
[3] $P\bar{3}$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a;2c$	$1b;2c$	$3\times2c$	$3\times2d$	$3e;6g$	$3f;6g$	$3\times6g$
[p] $P\bar{3}$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$; $p=$ prime >2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$1a$; $\frac{p-1}{2}\times2c$	$1b$; $\frac{p-1}{2}\times2c$	$p\times2c$	$p\times2d$	$3e$; $\frac{p-1}{2}\times6g$	$3f$; $\frac{p-1}{2}\times6g$	$p\times6g$
[3] $P\bar{3}$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;2d$	$1b;2d$	$2c;2\times2d$	$6g$	$3e;6g$	$3f;6g$	$3\times6g$
[7] $P\bar{3}$	$3\mathbf{a}+\mathbf{b}, -\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z$; $\pm(\frac{1}{7},\frac{3}{7},0)$; $\pm(\frac{3}{7},\frac{2}{7},0)$; $\pm(\frac{5}{7},\frac{1}{7},0)$	$1a;6g$	$1b;6g$	$2c;2\times6g$	$2d;2\times6g$	$3e;3\times6g$	$3f;3\times6g$	$7\times6g$
[7] $P\bar{3}$	$3\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z$; $\pm(\frac{2}{7},\frac{3}{7},0)$; $\pm(\frac{3}{7},\frac{1}{7},0)$; $\pm(\frac{1}{7},\frac{5}{7},0)$	$1a;6g$	$1b;6g$	$2c;2\times6g$	$2d;2\times6g$	$3e;3\times6g$	$3f;3\times6g$	$7\times6g$
[p] $P\bar{3}$	$q\mathbf{a}+r\mathbf{b}, -r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$; $p=$ prime $=q^2-qr+r^2=6n+1$; $q,r=1,2,\ldots$; $q>r$; $u=1,\ldots,p-1$	$\frac{1}{p}((q-r)x+ry)$, $\frac{1}{p}(-rx+qy), z$; $+(\frac{ur}{p},\frac{uq}{p},0)$	$1a$; $\frac{p-1}{6}\times6g$	$1b$; $\frac{p-1}{6}\times6g$	$2c$; $\frac{p-1}{3}\times6g$	$2d$; $\frac{p-1}{3}\times6g$	$3e$; $\frac{p-1}{2}\times6g$	$3f$; $\frac{p-1}{2}\times6g$	$p\times6g$
[4] $P\bar{3}$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a;3e$	$1b;3f$	$2c;6g$	$2d;6g$	$2\times6g$	$2\times6g$	$4\times6g$
[p^2] $P\bar{3}$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$; $p=$ prime $=6n-1$; $u,v=1,\ldots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$1a$; $\frac{p^2-1}{6}\times6g$	$1b$; $\frac{p^2-1}{6}\times6g$	$2c$; $\frac{p^2-1}{3}\times6g$	$2d$; $\frac{p^2-1}{3}\times6g$	$3e$; $\frac{p^2-1}{2}\times6g$	$3f$; $\frac{p^2-1}{2}\times6g$	$p^2\times6g$

$R\bar{3}$ No. 148 C_{3i}^{2}

HEXAGONAL AXES

	Axes	Coordinates	$3a$	$3b$	$6c$	$9d$	$9e$	$18f$
I Maximal *translationengleiche* subgroups								
[2] $R3$ (146)			$3a$	$3a$	$2\times3a$	$9b$	$9b$	$2\times9b$
[3] $P\bar{1}$ (2)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$ rhombo. axes: $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$x+z, -x+y+z, -y+z$ x, y, z	$1a$	$1h$	$2i$	$1b; 1c; 1d$	$1e; 1f; 1g$	$3\times2i$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[3] $P\bar{3}$ (147)			$1a; 2d$	$1b; 2d$	$2c; 2\times2d$	$3f; 6g$	$3e; 6g$	$3\times6g$
Enlarged unit cell, isomorphic								
[2] $R\bar{3}$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$3a; 3b$	$6c$	$2\times6c$	$18f$	$9d; 9e$	$2\times18f$
[2] $R\bar{3}$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$6c$	$3a; 3b$	$2\times6c$	$9d; 9e$	$18f$	$2\times18f$
[p] $R\bar{3}$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$ $p = \text{prime} = 6n-1; u = 1,\ldots,p-1$ $\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} = 6n+1; u = 1,\ldots,p-1$	$-x, -y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$3a; \frac{p-1}{2}\times6c$	$3b; \frac{p-1}{2}\times6c$	$p\times6c$	$9d; \frac{p-1}{2}\times18f$	$9e; \frac{p-1}{2}\times18f$	$p\times18f$
[7] $R\bar{3}$	$3\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z$; $\pm(\frac{1}{7},\frac{3}{7},0); \pm(\frac{5}{7},\frac{1}{7},0); \pm(\frac{3}{7},\frac{2}{7},0)$	$3a; 18f$	$3b; 18f$	$6c; 2\times18f$	$9d; 3\times18f$	$9e; 3\times18f$	$7\times18f$
[7] $R\bar{3}$	$\mathbf{a}+3\mathbf{b}$, $-3\mathbf{a}-2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(-2x+3y), \frac{1}{7}(-3x+y), z$; $\pm(\frac{1}{7},\frac{5}{7},0); \pm(\frac{2}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{1}{7},0)$	$3a; 18f$	$3b; 18f$	$6c; 2\times18f$	$9d; 3\times18f$	$9e; 3\times18f$	$7\times18f$
[p] $R\bar{3}$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$ $p = q^2-qr+r^2 = \text{prime} = 6n+1$; $q, r = 1, 2, \ldots;\ q \neq r;\ q+r = 3n+1$;	$\frac{1}{p}((q-r)x+ry)$, $\frac{1}{p}(-rx+qy), z; +(\frac{ur}{p}, \frac{uq}{p}, 0)$ $u = 1,\ldots,p-1$	$3a; \frac{p-1}{6}\times18f$	$3b; \frac{p-1}{6}\times18f$	$6c; \frac{p-1}{3}\times18f$	$9d; \frac{p-1}{2}\times18f$	$9e; \frac{p-1}{2}\times18f$	$p\times18f$
[4] $R\bar{3}$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z; +(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$3a; 9e$	$3b; 9d$	$6c; 18f$	$2\times18f$	$2\times18f$	$4\times18f$
[p^2] $R\bar{3}$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$ $p = \text{prime} = 6n-1;\ u, v = 1,\ldots,p-1$	$-\frac{1}{p}x, -\frac{1}{p}y, z;\ +(\frac{u}{p}, \frac{v}{p}, 0)$	$3a; \frac{p^2-1}{6}\times18f$	$3b; \frac{p^2-1}{6}\times18f$	$6c; \frac{p^2-1}{3}\times18f$	$9d; \frac{p^2-1}{2}\times18f$	$9e; \frac{p^2-1}{2}\times18f$	$p^2\times18f$

$P312$ No. 149

CONTINUED (*from next page*)

	Axes	Coordinates	$1a$	$1b$	$1c$ $2h$	$1d$ $2i$	$1e$ $3j$	$1f$ $3k$	$2g$ $6l$
[p] $P312$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2;\ u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$1a; \frac{p-1}{2}\times2g$	$1b; \frac{p-1}{2}\times2g$	$1c; \frac{p-1}{2}\times2h$ $p\times2h$	$1d; \frac{p-1}{2}\times2h$ $p\times2i$	$1e; \frac{p-1}{2}\times2i$ $3j; \frac{p-1}{2}\times6l$	$1f; \frac{p-1}{2}\times2i$ $3k; \frac{p-1}{2}\times6l$	$p\times2g$ $p\times6l$
[4] $P312$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$1a; 3j$	$1b; 3k$	$1e; 3j$ $2i; 6l$	$1f; 3k$ $2h; 6l$	$1c; 3j$ $2\times3j; 6l$	$1d; 3k$ $2\times3k; 6l$	$2g; 6l$ $4\times6l$
[p^2] $P312$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 4$;	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$ $u, v = 1,\ldots,p-1$	$1a$; $(p-1)\times3j$; $\frac{(p-1)(p-2)}{6}\times6l$	$1b$; $(p-1)\times3k$; $\frac{(p-1)(p-2)}{6}\times6l$	$1c(e^*)$; $(p-1)\times3j$; $\frac{(p-1)(p-2)}{6}\times6l$ $2h(i^*)$; $\frac{p^2-1}{3}\times6l$	$1d(f^*)$; $(p-1)\times3k$; $\frac{(p-1)(p-2)}{6}\times6l$ $2i(h^*)$; $\frac{p^2-1}{3}\times6l$	$1e(c^*)$; $(p-1)\times3j$; $\frac{(p-1)(p-2)}{6}\times6l$ $p\times3j$; $\frac{p(p-1)}{2}\times6l$	$1f(d^*)$; $(p-1)\times3k$; $\frac{(p-1)(p-2)}{6}\times6l$ $p\times3k$; $\frac{p(p-1)}{2}\times6l$	$2g; \frac{p^2-1}{3}\times6l$ $p^2\times6l$

* $p = 6n-1$

	Axes	Coordinates	1*a*	1*b*	1*c*	1*d*	1*e*	1*f*	2*g*	2*h*	2*i* 3*k*	3*j* 6*l*
I Maximal *translationengleiche* subgroups												
[2] $P3$ (143)			1*a*	1*a*	1*b*	1*b*	1*c*	1*c*	2×1*a*	2×1*b*	2×1*c* 3*d*	3*d* 2×3*d*
[3] $C121$ (5)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	2*a*	2*b*	2*a*	2*b*	2*a*	2*b*	4*c*	4*c*	4*c* 2*b*; 4*c*	2*a*; 4*c* 3×4*c*
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$										
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$										
II Maximal *klassengleiche* subgroups												
Enlarged unit cell, non-isomorphic												
[3] $R32$ (155)	**a**−**b**, **a**+2**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	3*a*; 6*c*	3*b*; 6*c*	9*d*	9*e*	9*d*	9*e*	3×6*c*	18*f*	18*f* 9*e*; 18*f*	9*d*; 18*f* 3×18*f*
[3] $R32$ (155)	**a**−**b**, **a**+2**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(2x-y)-\frac{1}{3}, \frac{1}{3}(x+y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	9*d*	9*e*	3*a*; 6*c*	3*b*; 6*c*	9*d*	9*e*	18*f*	3×6*c*	18*f* 9*e*; 18*f*	9*d*; 18*f* 3×18*f*
[3] $R32$ (155)	**a**−**b**, **a**+2**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(2x-y)+\frac{1}{3}, \frac{1}{3}(x+y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	9*d*	9*e*	9*d*	9*e*	3*a*; 6*c*	3*b*; 6*c*	18*f*	18*f*	3×6*c* 9*e*; 18*f*	9*d*; 18*f* 3×18*f*
[3] $R32$ (155)	2**a**+**b**, −**a**+**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	3*a*; 6*c*	3*b*; 6*c*	9*d*	9*e*	9*d*	9*e*	3×6*c*	18*f*	18*f* 9*e*; 18*f*	9*d*; 18*f* 3×18*f*
[3] $R32$ (155)	2**a**+**b**, −**a**+**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	9*d*	9*e*	9*d*	9*e*	3*a*; 6*c*	3*b*; 6*c*	18*f*	18*f*	3×6*c* 9*e*; 18*f*	9*d*; 18*f* 3×18*f*
[3] $R32$ (155)	2**a**+**b**, −**a**+**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	9*d*	9*e*	3*a*; 6*c*	3*b*; 6*c*	9*d*	9*e*	18*f*	3×6*c*	18*f* 9*e*; 18*f*	9*d*; 18*f* 3×18*f*
[3] $P3_212$ (153)	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	3*a*	3*b*	3*a*	3*b*	3*a*	3*b*	6*c*	6*c*	6*c* 3*b*; 6*c*	3*a*; 6*c* 3×6*c*
[3] $P3_112$ (151)	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	3*a*	3*b*	3*a*	3*b*	3*a*	3*b*	6*c*	6*c*	6*c* 3*b*; 6*c*	3*a*; 6*c* 3×6*c*
[3] $P321$ (150)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	1*a*; 2*d*	1*b*; 2*d*	3*e*	3*f*	3*e*	3*f*	2*c*; 2×2*d*	6*g*	6*g* 3*f*; 6*g*	3*e*; 6*g* 3×6*g*
[3] $P321$ (150)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	3*e*	3*f*	3*e*	3*f*	1*a*; 2*d*	1*b*; 2*d*	6*g*	6*g*	2*c*; 2×2*d* 3*f*; 6*g*	3*e*; 6*g* 3×6*g*
[3] $P321$ (150)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	3*e*	3*f*	1*a*; 2*d*	1*b*; 2*d*	3*e*	3*f*	6*g*	2*c*; 2×2*d*	6*g* 3*f*; 6*g*	3*e*; 6*g* 3×6*g*
Enlarged unit cell, isomorphic												
[2] $P312$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	1*a*; 1*b*	2*g*	1*c*; 1*d*	2*h*	1*e*; 1*f*	2*i*	2×2*g*	2×2*h*	2×2*i* 6*l*	3*j*; 3*k* 2×6*l*
[2] $P312$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*g*	1*a*; 1*b*	2*h*	1*c*; 1*d*	2*i*	1*e*; 1*f*	2×2*g*	2×2*h*	2×2*i* 3*j*; 3*k*	6*l* 2×6*l*
[3] $P312$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	1*a*; 2*g*	1*b*; 2*g*	1*c*; 2*h*	1*d*; 2*h*	1*e*; 2*i*	1*f*; 2*i*	3×2*g*	3×2*h*	3×2*i* 3*k*; 6*l*	3*j*; 6*l* 3×6*l*

Continued on preceding page

$P321$ No. 150 D_3^2

	Axes	Coordinates	Wyckoff positions 1*a*	1*b*	2*c*	2*d*	3*e*	3*f*	6*g*
I Maximal *translationengleiche* subgroups									
[2] $P3$ (143)			1*a*	1*a*	2×1*a*	1*b*; 1*c*	3*d*	3*d*	2×3*d*
[3] $C121$ (5)	$2\mathbf{a}+\mathbf{b}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z$;	2*a*	2*b*	4*c*	4*c*	2*a*; 4*c*	2*b*; 4*c*	3×4*c*
conjugate:	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$;							
conjugate:	$\mathbf{a}+2\mathbf{b}$, $-\mathbf{a}$, $\mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z$;							
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[3] $P3_221$ (154)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	3*a*	3*b*	6*c*	6*c*	3*a*; 6*c*	3*b*; 6*c*	3×6*c*
[3] $P3_121$ (152)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	3*a*	3*b*	6*c*	6*c*	3*a*; 6*c*	3*b*; 6*c*	3×6*c*
[3] $P312$ (149)	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	1*a*; 1*c*; 1*e*	1*b*; 1*d*; 1*f*	2*g*; 2*h*; 2*i*	6*l*	3×3*j*	3×3*k*	3×6*l*
Enlarged unit cell, isomorphic									
[2] $P321$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	1*a*; 1*b*	2*c*	2×2*c*	2×2*d*	3*e*; 3*f*	6*g*	2×6*g*
[2] $P321$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*c*	1*a*; 1*b*	2×2*c*	2×2*d*	6*g*	3*e*; 3*f*	2×6*g*
[3] $P321$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	1*a*; 2*c*	1*b*; 2*c*	3×2*c*	3×2*d*	3*e*; 6*g*	3*f*; 6*g*	3×6*g*
[p] $P321$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p=$ prime >2; $u=1,\ldots,p-1$	1*a*; $\frac{p-1}{2}\times 2c$	1*b*; $\frac{p-1}{2}\times 2c$	$p\times 2c$	$p\times 2d$	3*e*; $\frac{p-1}{2}\times 6g$	3*f*; $\frac{p-1}{2}\times 6g$	$p\times 6g$
[4] $P321$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	1*a*; 3*e*	1*b*; 3*f*	2*c*; 6*g*	2*d*; 6*g*	2×3*e*; 6*g*	2×3*f*; 6*g*	4×6*g*
[p^2] $P321$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ $p=$ prime $\neq 3$; $u,v=1,\ldots,p-1$	1*a*; $(p-1)\times 3e$; $\frac{(p-1)(p-2)}{6}\times 6g$	1*b*; $(p-1)\times 3f$; $\frac{(p-1)(p-2)}{6}\times 6g$	2*c*; $\frac{p^2-1}{3}\times 6g$	2*d*; $\frac{p^2-1}{3}\times 6g$	$p\times 3e$; $\frac{p(p-1)}{2}\times 6g$	$p\times 3f$; $\frac{p(p-1)}{2}\times 6g$	$p^2\times 6g$

D_3^3 No. 151 $P3_112$

	Axes	Coordinates	Wyckoff positions 3*a*	3*b*	6*c*
I Maximal *translationengleiche* subgroups					
[2] $P3_1$ (144)			$3a$	$3a$	$2\times3a$
[3] $C121$ (5)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z+\frac{1}{3}$	$2a; 4c$	$2b; 4c$	$3\times4c$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$			
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(-x-y), \frac{1}{2}(x-y), z-\frac{1}{3}$			
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[3] $P3_121$ (152)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$3a; 6c$	$3b; 6c$	$3\times6c$
[3] $P3_121$ (152)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y)-\frac{1}{3}, \frac{1}{3}(x+y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$3a; 6c$	$3b; 6c$	$3\times6c$
[3] $P3_121$ (152)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y)+\frac{1}{3}, \frac{1}{3}(x+y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$3a; 6c$	$3b; 6c$	$3\times6c$
Enlarged unit cell, isomorphic					
[2] $P3_212$ (153)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$3a; 3b$	$6c$	$2\times6c$
[2] $P3_212$ (153)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$	$6c$	$3a; 3b$	$2\times6c$
[5] $P3_212$ (153)	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0, 0, \frac{1}{5}); \pm(0, 0, \frac{2}{5})$	$3a; 2\times6c$	$3b; 2\times6c$	$5\times6c$
[p] $P3_212$ (153)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$ $p = \text{prime} = 6n-1;\ u = 1, \ldots, p-1$	$3a; \frac{p-1}{2}\times6c$	$3b; \frac{p-1}{2}\times6c$	$p\times6c$
[7] $P3_112$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z; \pm(0, 0, \frac{1}{7}); \pm(0, 0, \frac{2}{7}); \pm(0, 0, \frac{3}{7})$	$3a; 3\times6c$	$3b; 3\times6c$	$7\times6c$
[p] $P3_112$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$ $p = \text{prime} = 6n+1;\ u = 1, \ldots, p-1$	$3a; \frac{p-1}{2}\times6c$	$3b; \frac{p-1}{2}\times6c$	$p\times6c$
[4] $P3_112$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0); +(0, \frac{1}{2}, 0); +(\frac{1}{2}, \frac{1}{2}, 0)$	$2\times3a; 6c$	$2\times3b; 6c$	$4\times6c$
[p^2] $P3_112$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$ $p = \text{prime} \neq 3;\ u, v = 1, \ldots, p-1$	$p\times3a; \frac{p(p-1)}{2}\times6c$	$p\times3b; \frac{p(p-1)}{2}\times6c$	$p^2\times6c$

$P3_121$ No. 152 D_3^4

	Axes	Coordinates	Wyckoff positions		
			$3a$	$3b$	$6c$
I Maximal *translationengleiche* subgroups					
[2] $P3_1$ (144)			$3a$	$3a$	$2\times3a$
[3] $C121$ (5)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2a; 4c$	$2b; 4c$	$3\times4c$
conjugate:	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z+\frac{1}{3}$			
conjugate:	$\mathbf{a}+2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z-\frac{1}{3}$			
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[3] $P3_112$ (151)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$3\times3a$	$3\times3b$	$3\times6c$
Enlarged unit cell, isomorphic					
[2] $P3_221$ (154)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$3a; 3b$	$6c$	$2\times6c$
[2] $P3_221$ (154)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$	$6c$	$3a; 3b$	$2\times6c$
[5] $P3_221$ (154)	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0, 0, \frac{1}{5}); \pm(0, 0, \frac{2}{5})$	$3a; 2\times6c$	$3b; 2\times6c$	$5\times6c$
[p] $P3_221$ (154)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$3a; \frac{p-1}{2}\times6c$	$3b; \frac{p-1}{2}\times6c$	$p\times6c$
	$p = \text{prime} = 6n-1;\ u = 1, \ldots, p-1$				
[7] $P3_121$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z; \pm(0, 0, \frac{1}{7}); \pm(0, 0, \frac{2}{7}); \pm(0, 0, \frac{3}{7})$	$3a; 3\times6c$	$3b; 3\times6c$	$7\times6c$
[p] $P3_121$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$3a; \frac{p-1}{2}\times6c$	$3b; \frac{p-1}{2}\times6c$	$p\times6c$
	$p = \text{prime} = 6n+1;\ u = 1, \ldots, p-1$				
[4] $P3_121$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0); +(0, \frac{1}{2}, 0); +(\frac{1}{2}, \frac{1}{2}, 0)$	$2\times3a; 6c$	$2\times3b; 6c$	$4\times6c$
[p^2] $P3_121$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$	$p\times3a; \frac{p(p-1)}{2}\times6c$	$p\times3b; \frac{p(p-1)}{2}\times6c$	$p^2\times6c$
	$p = \text{prime} \neq 3;\ u, v = 1, \ldots, p-1$				

D_3^5 No. 153 $P3_212$

Axes	Coordinates		Wyckoff positions		
			$3a$	$3b$	$6c$
I Maximal *translationengleiche* subgroups					
[2] $P3_2$ (145)			$3a$	$3a$	$2\times3a$
[3] $C121$ (5)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z-\frac{1}{3}$	$2a;4c$	$2b;4c$	$3\times4c$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$			
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(-x-y), \frac{1}{2}(x-y), z+\frac{1}{3}$			
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[3] $P3_221$ (154)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), z; \pm(\frac{1}{3}, \frac{2}{3}, 0)$	$3a;6c$	$3b;6c$	$3\times6c$
[3] $P3_221$ (154)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y)-\frac{1}{3}, \frac{1}{3}(x+y), z; \pm(\frac{1}{3}, \frac{2}{3}, 0)$	$3a;6c$	$3b;6c$	$3\times6c$
[3] $P3_221$ (154)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y)+\frac{1}{3}, \frac{1}{3}(x+y), z; \pm(\frac{1}{3}, \frac{2}{3}, 0)$	$3a;6c$	$3b;6c$	$3\times6c$
Enlarged unit cell, isomorphic					
[2] $P3_112$ (151)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$3a;3b$	$6c$	$2\times6c$
[2] $P3_112$ (151)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0, 0, \frac{1}{2})$	$6c$	$3a;3b$	$2\times6c$
[5] $P3_112$ (151)	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0, 0, \frac{1}{5}); \pm(0, 0, \frac{2}{5})$	$3a;2\times6c$	$3b;2\times6c$	$5\times6c$
[p] $P3_112$ (151)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$3a;\frac{p-1}{2}\times6c$	$3b;\frac{p-1}{2}\times6c$	$p\times6c$
	$p = \text{prime} = 6n-1;\ u = 1, \ldots, p-1$				
[7] $P3_212$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z; \pm(0, 0, \frac{1}{7}); \pm(0, 0, \frac{2}{7}); \pm(0, 0, \frac{3}{7})$	$3a;3\times6c$	$3b;3\times6c$	$7\times6c$
[p] $P3_212$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$3a;\frac{p-1}{2}\times6c$	$3b;\frac{p-1}{2}\times6c$	$p\times6c$
	$p = \text{prime} = 6n+1;\ u = 1, \ldots, p-1$				
[4] $P3_212$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0); +(0, \frac{1}{2}, 0); +(\frac{1}{2}, \frac{1}{2}, 0)$	$2\times3a;6c$	$2\times3b;6c$	$4\times6c$
[p^2] $P3_212$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$	$p\times3a;\frac{p(p-1)}{2}\times6c$	$p\times3b;\frac{p(p-1)}{2}\times6c$	$p^2\times6c$
	$p = \text{prime} \neq 3;\ u, v = 1, \ldots, p-1$				

$P3_221$ No. 154 D_3^6

Axes		Coordinates	Wyckoff positions 3*a*	3*b*	6*c*
I Maximal *translationengleiche* subgroups					
[2] $P3_2$ (145)			$3a$	$3a$	$2\times3a$
[3] $C121$ (5)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$	$2a;4c$	$2b;4c$	$3\times4c$
conjugate:	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z-\frac{1}{3}$			
conjugate:	$\mathbf{a}+2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z+\frac{1}{3}$			
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[3] $P3_212$ (153)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$3\times3a$	$3\times3b$	$3\times6c$
Enlarged unit cell, isomorphic					
[2] $P3_121$ (152)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$3a;3b$	$6c$	$2\times6c$
[2] $P3_121$ (152)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$6c$	$3a;3b$	$2\times6c$
[5] $P3_121$ (152)	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$	$3a;2\times6c$	$3b;2\times6c$	$5\times6c$
[p] $P3_121$ (152)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$3a;\frac{p-1}{2}\times6c$	$3b;\frac{p-1}{2}\times6c$	$p\times6c$
	$p = \text{prime} = 6n-1;\ u = 1,\ldots,p-1$				
[7] $P3_221$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z; \pm(0,0,\frac{1}{7}); \pm(0,0,\frac{2}{7}); \pm(0,0,\frac{3}{7})$	$3a;3\times6c$	$3b;3\times6c$	$7\times6c$
[p] $P3_221$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$3a;\frac{p-1}{2}\times6c$	$3b;\frac{p-1}{2}\times6c$	$p\times6c$
	$p = \text{prime} = 6n+1;\ u = 1,\ldots,p-1$				
[4] $P3_221$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$2\times3a;6c$	$2\times3b;6c$	$4\times6c$
[p^2] $P3_221$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$p\times3a;\frac{p(p-1)}{2}\times6c$	$p\times3b;\frac{p(p-1)}{2}\times6c$	$p^2\times6c$
	$p = \text{prime} \neq 3;\ u,v = 1,\ldots,p-1$				

D_3^7 No. 155 $R32$

HEXAGONAL AXES

	Axes	Coordinates	Wyckoff positions $3a$	$3b$	$6c$	$9d$	$9e$	$18f$
I Maximal *translationengleiche* subgroups								
[2] $R3$ (146)			$3a$	$3a$	$2\times3a$	$9b$	$9b$	$2\times9b$
[3] $C121$ (5)	$\tfrac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c})$, $\mathbf{b}$, $\tfrac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\tfrac{1}{2}x-z, -\tfrac{1}{2}x+y, x+z$	$2a$	$2b$	$4c$	$2a;\,4c$	$2b;\,4c$	$3\times4c$
conjugate:	$\tfrac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c})$, $-\mathbf{a}-\mathbf{b}$, $\tfrac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$	$-\tfrac{1}{2}x+\tfrac{1}{2}y-z, -\tfrac{1}{2}(x+y), -x+y+z$						
conjugate:	$\tfrac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c})$, $\mathbf{a}$, $\tfrac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	$-\tfrac{1}{2}y-z, x-\tfrac{1}{2}y, -y+z$						
alternative:	$\tfrac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c})$, $\mathbf{b}$, $\mathbf{c}$	$\tfrac{3}{2}x, -\tfrac{1}{2}x+y, x+z$						
or	$\tfrac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c})$, $-\mathbf{a}-\mathbf{b}$, $\mathbf{c}$	$\tfrac{3}{2}(-x+y), -\tfrac{1}{2}(x+y), -x+y+z$						
or	$\tfrac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c})$, $\mathbf{a}$, $\mathbf{c}$	$-\tfrac{3}{2}y, x-\tfrac{1}{2}y, -y+z$						
alternative:	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{b}$, $-\tfrac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\tfrac{1}{2}x-z, \tfrac{1}{2}x-y, -3z$						
or	$-\mathbf{a}+\mathbf{b}$, $\mathbf{a}+\mathbf{b}$, $\tfrac{1}{3}(\mathbf{a}-\mathbf{b}-\mathbf{c})$	$\tfrac{1}{2}(-x+y)-z, \tfrac{1}{2}(x+y), -3z$						
or	$-\mathbf{a}-2\mathbf{b}$, $-\mathbf{a}$, $\tfrac{1}{3}(\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$-\tfrac{1}{2}y-z, -x+\tfrac{1}{2}y, -3z$						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[3] $P3_221$ (154)	3 conjugate subgroups	$x+\tfrac{1}{3}, y+\tfrac{1}{3}, z$	$3a$	$3b$	$6c$	$3a;6c$	$3b;6c$	$3\times6c$
[3] $P3_121$ (152)	3 conjugate subgroups	$x-\tfrac{1}{3}, y-\tfrac{1}{3}, z$	$3a$	$3b$	$6c$	$3a;6c$	$3b;6c$	$3\times6c$
[3] $P321$ (150)	3 conjugate subgroups		$1a;\,2d$	$1b;\,2d$	$2c;2\times2d$	$3e;6g$	$3f;6g$	$3\times6g$
Enlarged unit cell, isomorphic								
[2] $R32$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x,-y,\tfrac{1}{2}z;\ +(0,0,\tfrac{1}{2})$	$3a;3b$	$6c$	$2\times6c$	$9d;9e$	$18f$	$2\times18f$
[2] $R32$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x,-y,\tfrac{1}{2}z+\tfrac{1}{4};\ +(0,0,\tfrac{1}{2})$	$6c$	$3a;3b$	$2\times6c$	$18f$	$9d;9e$	$2\times18f$
[5] $R32$	$-\mathbf{a}, -\mathbf{b}, 5\mathbf{c}$	$-x,-y,\tfrac{1}{5}z;\ \pm(0,0,\tfrac{1}{5})\ \pm(0,0,\tfrac{2}{5})$	$3a;2\times6c$	$3b;2\times6c$	$5\times6c$	$9d;2\times18f$	$9e;2\times18f$	$5\times18f$
[p] $R32$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$; $p = \text{prime} = 6n-1$; $u = 1,\ldots,p-1$	$-x,-y,\tfrac{1}{p}z;\ +(0,0,\tfrac{u}{p})$	$3a;\tfrac{p-1}{2}\times6c$	$3b;\tfrac{p-1}{2}\times6c$	$p\times6c$	$9d;\tfrac{p-1}{2}\times18f$	$9e;\tfrac{p-1}{2}\times18f$	$p\times18f$
	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$; $p = \text{prime} = 6n+1$; $u = 1,\ldots,p-1$	$x,y,\tfrac{1}{p}z;\ +(0,0,\tfrac{u}{p})$						
[4] $R32$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\tfrac{1}{2}x,-\tfrac{1}{2}y,z;+(\tfrac{1}{2},0,0);\ +(0,\tfrac{1}{2},0);\ +(\tfrac{1}{2},\tfrac{1}{2},0)$	$3a;9d$	$3b;9e$	$6c;18f$	$2\times9d;18f$	$2\times9e;18f$	$4\times18f$
[p^2] $R32$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$; $p=\text{prime}=6n-1$; $u,v=1,\ldots,p-1$	$-\tfrac{1}{p}x,-\tfrac{1}{p}y,z;+(\tfrac{u}{p},\tfrac{v}{p},0)$	$3a;(p-1)\times9d;\tfrac{(p-1)(p-2)}{6}\times18f$	$3b;(p-1)\times9e;\tfrac{(p-1)(p-2)}{6}\times18f$	$6c;\tfrac{p^2-1}{3}\times18f$	$p\times9d;\tfrac{p(p-1)}{2}\times18f$	$p\times9e;\tfrac{p(p-1)}{2}\times18f$	$p^2\times18f$
	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$; $p=\text{prime}=6n+1$; $u,v=1,\ldots,p-1$	$\tfrac{1}{p}x,\tfrac{1}{p}y,z;\ +(\tfrac{u}{p},\tfrac{v}{p},0)$						

$P3m1$ No. 156 C_{3v}^1

	Axes	Coordinates	Wyckoff positions 1a	1b	1c	3d	6e
I Maximal *translationengleiche* subgroups							
[2] $P3$ (143)			1a	1b	1c	3d	2×3d
[3] $C1m1$ (8)	**2a+b**, **b**, **c**	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	2a	2a	2a	2a; 4b	3×4b
conjugate:	**a−b**, **a+b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$					
conjugate:	**a+2b**, **−a**, **c**	$\frac{1}{2}y, -x+\frac{1}{2}y, z$					
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, non-isomorphic							
[2] $P3c1$ (158)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2a	2b	2c	6d	2×6d
[3] $P31m$ (157)	2**a+b**, −**a+b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	1a; 2b	3c	3c	3c; 6d	3×6d
[3] $P31m$ (157)	2**a+b**, −**a+b**, **c**	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	3c	1a; 2b	3c	3c; 6d	3×6d
[3] $P31m$ (157)	2**a+b**, −**a+b**, **c**	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	3c	3c	1a; 2b	3c; 6d	3×6d
Enlarged unit cell, isomorphic							
[2] $P3m1$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2×1a	2×1b	2×1c	2×3d	2×6e
[3] $P3m1$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	3×1a	3×1b	3×1c	3×3d	3×6e
[p] $P3m1$	**a**, **b**, p**c**; p = prime; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	p×1a	p×1b	p×1c	p×3d	p×6e
[4] $P3m1$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	1a; 3d	1c; 3d	1b; 3d	2×3d; 6e	4×6e
[p^2] $P3m1$	p**a**, p**b**, **c**; p = prime ≠ 3; $u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	1a; $(p-1)\times 3d$; $\frac{(p-1)(p-2)}{6}\times 6e$	1b(c*); $(p-1)\times 3d$; $\frac{(p-1)(p-2)}{6}\times 6e$	1c(b*); $(p-1)\times 3d$; $\frac{(p-1)(p-2)}{6}\times 6e$	$p\times 3d$; $\frac{p(p-1)}{2}\times 6e$	$p^2\times 6e$

* $p = 3n-1$

C_{3v}^2 No. 157 $P31m$

	Axes	Coordinates	Wyckoff positions $1a$	$2b$	$3c$	$6d$
I Maximal *translationengleiche* subgroups						
[2] $P3$ (143)			$1a$	$1b; 1c$	$3d$	$2\times 3d$
[3] $C1m1$ (8)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$2a$	$4b$	$2a; 4b$	$3\times 4b$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$				
conjugate:	$\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x+y), \frac{1}{2}(-x+y), z$				
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[3] $R3m$ (160)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times 3a$	$18c$	$3\times 9b$	$3\times 18c$
[3] $R3m$ (160)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, 3\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times 3a$	$18c$	$3\times 9b$	$3\times 18c$
[2] $P31c$ (159)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$	$2\times 2b$	$6c$	$2\times 6c$
[3] $P3m1$ (156)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), z; \pm(\frac{2}{3},\frac{1}{3},0)$	$1a; 1b; 1c$	$6e$	$3\times 3d$	$3\times 6e$
Enlarged unit cell, isomorphic						
[2] $P31m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2\times 1a$	$2\times 2b$	$2\times 3c$	$2\times 6d$
[3] $P31m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times 1a$	$3\times 2b$	$3\times 3c$	$3\times 6d$
[p] $P31m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime}; u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times 1a$	$p\times 2b$	$p\times 3c$	$p\times 6d$
[4] $P31m$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$1a; 3c$	$2b; 6d$	$2\times 3c; 6d$	$4\times 6d$
[p^2] $P31m$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} \neq 3; u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$1a; (p-1)\times 3c; \frac{(p-1)(p-2)}{6}\times 6d$	$2b; \frac{p^2-1}{3}\times 6d$	$p\times 3c; \frac{p(p-1)}{2}\times 6d$	$p^2\times 6d$

$P3c1$ No. 158 C_{3v}^3

	Axes	Coordinates	Wyckoff positions $2a$	$2b$	$2c$	$6d$
I Maximal *translationengleiche* subgroups						
[2] $P3$ (143)			$2\times1a$	$2\times1b$	$2\times1c$	$2\times3d$
[3] $C1c1$ (9)	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	$4a$	$4a$	$4a$	$3\times4a$
conjugate:	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$				
conjugate:	$\mathbf{a}+2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z$				
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[3] $P31c$ (159)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$2a; 2\times2b$	$6c$	$6c$	$3\times6c$
[3] $P31c$ (159)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$6c$	$6c$	$2a; 2\times2b$	$3\times6c$
[3] $P31c$ (159)	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$6c$	$2a; 2\times2b$	$6c$	$3\times6c$
Enlarged unit cell, isomorphic						
[3] $P3c1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times2c$	$3\times6d$
[p] $P3c1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$p\times2a$	$p\times2b$	$p\times2c$	$p\times6d$
	$p=$ prime >2; $u=1,\ldots,p-1$					
[4] $P3c1$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0); +(0, \frac{1}{2}, 0); +(\frac{1}{2}, \frac{1}{2}, 0)$	$2a; 6d$	$2c; 6d$	$2b; 6d$	$4\times6d$
[p^2] $P3c1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$	$2a; \frac{p^2-1}{3}\times6d$	$2b(c^*); \frac{p^2-1}{3}\times6d$	$2c(b^*); \frac{p^2-1}{3}\times6d$	$p^2\times6d$
	$p=$ prime $\neq 3$; $u, v=1,\ldots,p-1$					

* $p=3n-1$

C_{3v}^4 No. 159 $P31c$

Axes	Coordinates	Wyckoff positions		
		$2a$	$2b$	$6c$
I Maximal *translationengleiche* subgroups				
[2] $P3$ (143)		$2\times1a$	$1b; 1c$	$2\times3d$
[3] $C1c1$ (9) **a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$4a$	$4a$	$3\times4a$
conjugate: **b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$			
conjugate: −**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$			
II Maximal *klassengleiche* subgroups				
Enlarged unit cell, non-isomorphic				
[3] $P3c1$ (158) 2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$2a; 2b; 2c$	$6d$	$3\times6d$
[3] $R3c$ (161) **a**−**b**, **a**+2**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times6a$	$18b$	$3\times18b$
[3] $R3c$ (161) 2**a**+**b**, −**a**+**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times6a$	$18b$	$3\times18b$
Enlarged unit cell, isomorphic				
[3] $P31c$ **a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times6c$
[p] $P31c$ **a**, **b**, p**c** (p = prime > 2; $u = 1, \ldots, p-1$)	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times2a$	$p\times2b$	$p\times6c$
[4] $P31c$ 2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$2a; 6c$	$2b; 6c$	$4\times6c$
[p^2] $P31c$ p**a**, p**b**, **c** (p = prime $\neq 3$; $u, v = 1, \ldots, p-1$)	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$	$2a; \frac{p^2-1}{3}\times6c$	$2b; \frac{p^2-1}{3}\times6c$	$p^2\times6c$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 160, p. 644.

$R3m$ No. 160 C_{3v}^{5}

HEXAGONAL AXES

	Axes	Coordinates	Wyckoff positions $3a$	$9b$	$18c$
I Maximal *translationengleiche* subgroups					
[2] $R3$ (146)			$3a$	$9b$	$2\times 9b$
[3] $C1m1$ (8)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c}), \mathbf{b}, \frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}x-z, -\frac{1}{2}x+y, x+z$	$2a$	$2a; 4b$	$3\times 4b$
conjugate:	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \frac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$	$-\frac{1}{2}x+\frac{1}{2}y-z, -\frac{1}{2}x-\frac{1}{2}y, -x+y+z$			
conjugate:	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	$-\frac{1}{2}y-z, x-\frac{1}{2}y, -y+z$			
alternative:	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c}), \mathbf{b}, \mathbf{c}$	$\frac{3}{2}x, -\frac{1}{2}x+y, x+z$			
or	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \mathbf{c}$	$\frac{3}{2}(-x+y), -\frac{1}{2}(x+y), -x+y+z$			
or	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \mathbf{c}$	$-\frac{3}{2}y, x-\frac{1}{2}y, -y+z$			
alternative:	$2\mathbf{a}+\mathbf{b}, -\mathbf{b}, -\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}x-z, \frac{1}{2}x-y, -3z$			
or	$-\mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{b}, \frac{1}{3}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\frac{1}{3}(\mathbf{a}-\mathbf{b}-\mathbf{c})$	$\frac{1}{2}(-x+y)-z, \frac{1}{2}(x+y), -3z$			
or	$-\mathbf{a}-2\mathbf{b}, -\mathbf{a}, \frac{1}{3}(\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$-\frac{1}{2}y-z, -x+\frac{1}{2}y, -3z$			
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[3] $P3m1$ (156)			$1a; 1b; 1c$	$3\times 3d$	$3\times 6e$
Enlarged unit cell, non-isomorphic					
[2] $R3c$ (161)	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$6a$	$18b$	$2\times 18b$
Enlarged unit cell, isomorphic					
[2] $R3m$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2\times 3a$	$2\times 9b$	$2\times 18c$
[p] $R3m$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$ $p = \text{prime} = 3n-1;\ u = 1,\ldots,p-1$	$-x, -y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times 3a$	$p\times 9b$	$p\times 18c$
	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p = \text{prime} = 6n+1;\ u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$			
[4] $R3m$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z;\ +(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);\ +(\frac{1}{2},\frac{1}{2},0)$	$3a; 9b$	$2\times 9b; 18c$	$4\times 18c$
[p^2] $R3m$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$ $p = \text{prime} = 3n-1;\ u,v = 1,\ldots,p-1$	$-\frac{1}{p}x, -\frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$	$3a; (p-1)\times 9b;$ $\frac{(p-1)(p-2)}{6}\times 18c$	$p\times 9b;$ $\frac{p(p-1)}{2}\times 18c$	$p^2\times 18c$
	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} = 6n+1;\ u,v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$			

C_{3v}^{6} No. 161 $R3c$

HEXAGONAL AXES

Axes		Coordinates	Wyckoff positions 6*a*	18*b*
I Maximal *translationengleiche* subgroups				
[2] $R3$ (146)			$2\times3a$	$2\times9b$
[3] $C1c1$ (9)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c}), \mathbf{b}, \mathbf{c}$	$\frac{3}{2}x, -\frac{1}{2}x+y, x+z$	$4a$	$3\times4a$
conjugate:	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \mathbf{c}$	$\frac{3}{2}(-x+y), -\frac{1}{2}(x+y), -x+y+z$		
conjugate:	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \mathbf{c}$	$-\frac{3}{2}y, x-\frac{1}{2}y, -y+z$		
alternative:	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, -\frac{2}{3}(2\mathbf{a}+\mathbf{b})+\frac{1}{3}\mathbf{c}$	$\frac{1}{2}x+2z, -\frac{1}{2}x+y, 3z$		
or	$-\mathbf{a}+\mathbf{b}, -\mathbf{a}-\mathbf{b}, \frac{2}{3}(\mathbf{a}-\mathbf{b})+\frac{1}{3}\mathbf{c}$	$\frac{1}{2}(-x+y)+2z, -\frac{1}{2}(x+y), 3z$		
or	$-\mathbf{a}-2\mathbf{b}, \mathbf{a}, \frac{2}{3}(\mathbf{a}+2\mathbf{b})+\frac{1}{3}\mathbf{c}$	$-\frac{1}{2}y+2z, x-\frac{1}{2}y, 3z$		
II Maximal *klassengleiche* subgroups				
Loss of centring translations				
[3] $P3c1$ (158)			$2a; 2b; 2c$	$3\times6d$
Enlarged unit cell, isomorphic				
[5] $R3c$	$-\mathbf{a}, -\mathbf{b}, 5\mathbf{c}$	$-x, -y, \frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$	$5\times6a$	$5\times18b$
[p] $R3c$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$	$-x, -y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	$p\times6a$	$p\times18b$
	p = prime = $6n-1$; $u = 1,\ldots,p-1$			
	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$		
	p = prime = $6n+1$; $u = 1,\ldots,p-1$			
[4] $R3c$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z; +(\frac{1}{2},0,0); (0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$6a; 18b$	$4\times18b$
[p^2] $R3c$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$	$-\frac{1}{p}x, -\frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$6a; \frac{p^2-1}{3}\times18b$	$p^2\times18b$
	p = prime = $3n-1$; $u,v = 1,\ldots,p-1$			
	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z +(\frac{u}{p},\frac{v}{p},0)$		
	p = prime = $6n+1$; $u,v = 1,\ldots,p-1$			

$P\bar{3}1m$ No. 162 $P\bar{3}12/m$ D_{3d}^1

Subgroup	Axes	Coordinates	Wyckoff positions $1a$ $3g$	 $1b$ $4h$	 $2c$ $6i$	 $2d$ $6j$	 $2e$ $6k$	 $3f$ $12l$
I Maximal *translationengleiche* subgroups								
[2] $P31m$ (157)			$1a$ $3c$	$1a$ $2\times 2b$	$2b$ $6d$	$2b$ $6d$	$2\times 1a$ $2\times 3c$	$3c$ $2\times 6d$
[2] $P312$ (149)			$1a$ $3k$	$1b$ $2h$; $2i$	$1c$; $1e$ $2\times 3j$	$1d$; $1f$ $2\times 3k$	$2g$ $6l$	$3j$ $2\times 6l$
[2] $P\bar{3}$ (147)			$1a$ $3f$	$1b$ $2\times 2d$	$2d$ $6g$	$2d$ $6g$	$2c$ $6g$	$3e$ $2\times 6g$
[3] $C12/m1$ (12)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$2a$ $2d$; $4f$	$2c$ $8j$	$4g$ $4g$; $8j$	$4h$ $4h$; $8j$	$4i$ $4i$; $8j$	$2b$; $4e$ $3\times 8j$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$						
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P\bar{3}1c$ (163)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2b$ $6h$	$2a$ $2\times 4f$	$4f$ $12i$	$2c$; $2d$ $2\times 6h$	$4e$ $12i$	$6g$ $2\times 12i$
[2] $P\bar{3}1c$ (163)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2a$ $6g$	$2b$ $2\times 4f$	$2c$; $2d$ $2\times 6h$	$4f$ $12i$	$4e$ $12i$	$6h$ $2\times 12i$
[3] $R\bar{3}m$ (166)	**a**−**b**, **a**+2**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3a$; $6c$ $9d$; $18h$	$3b$; $6c$ $36i$	$18f$ $18f$; $36i$	$18g$ $18g$; $36i$	$3\times 6c$ $3\times 18h$	$9e$; $18h$ $3\times 36i$
[3] $R\bar{3}m$ (166)	2**a**+**b**, −**a**+**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3a$; $6c$ $9d$; $18h$	$3b$; $6c$ $36i$	$18f$ $18f$; $36i$	$18g$ $18g$; $36i$	$3\times 6c$ $3\times 18h$	$9e$; $18h$ $3\times 36i$
[3] $P\bar{3}m1$ (164)	**a**−**b**, **a**+2**b**, **c**	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), z$; $\pm(\frac{2}{3},\frac{1}{3},0)$	$1a$; $2d$ $3f$; $6i$	$1b$; $2d$ $12j$	$6g$ $6g$; $12j$	$6h$ $6h$; $12j$	$2c$; $2\times 2d$ $3\times 6i$	$3e$; $6i$ $3\times 12j$
Enlarged unit cell, isomorphic								
[2] $P\bar{3}1m$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a$; $1b$ $6k$	$2e$ $2\times 4h$	$2c$; $2d$ $6i$; $6j$	$4h$ $12l$	$2\times 2e$ $2\times 6k$	$3f$; $3g$ $2\times 12l$
[2] $P\bar{3}1m$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2e$ $3f$; $3g$	$1a$; $1b$ $2\times 4h$	$4h$ $12l$	$2c$; $2d$ $6i$; $6j$	$2\times 2e$ $2\times 6k$	$6k$ $2\times 12l$
[3] $P\bar{3}1m$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a$; $2e$ $3g$; $6k$	$1b$; $2e$ $3\times 4h$	$2c$; $4h$ $6i$; $12l$	$2d$; $4h$ $6j$; $12l$	$3\times 2e$ $3\times 6k$	$3f$; $6k$ $3\times 12l$
[p] $P\bar{3}1m$	**a**, **b**, p**c** p = prime > 2; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$1a$; $\frac{p-1}{2}\times 2e$ $3g$; $\frac{p-1}{2}\times 6k$	$1b$; $\frac{p-1}{2}\times 2e$ $p\times 4h$	$2c$; $\frac{p-1}{2}\times 4h$ $6i$; $\frac{p-1}{2}\times 12l$	$2d$; $\frac{p-1}{2}\times 4h$ $6j$; $\frac{p-1}{2}\times 12l$	$p\times 2e$ $p\times 6k$	$3f$; $\frac{p-1}{2}\times 6k$ $p\times 12l$
[4] $P\bar{3}1m$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a$; $3f$ $6j$; $6k$	$1b$; $3g$ $4h$; $12l$	$2c$; $6i$ $2\times 6i$; $12l$	$2d$; $6j$ $2\times 6j$; $12l$	$2e$; $6k$ $2\times 6k$; $12l$	$6i$; $6k$ $4\times 12l$
[p^2] $P\bar{3}1m$	p**a**, p**b**, **c** p = prime > 4; $u, v = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$1a$; $\frac{p-1}{2}\times 6i$; $\frac{p-1}{2}\times 6k$; $\frac{(p-1)(p-5)}{12}\times 12l$ $3g$; $\frac{p-1}{2}\times 6j$; $\frac{p-1}{2}\times 6k$; $\frac{(p-1)^2}{4}\times 12l$	$1b$; $\frac{p-1}{2}\times 6j$; $\frac{p-1}{2}\times 6k$; $\frac{(p-1)(p-5)}{12}\times 12l$ $4h$; $\frac{p^2-1}{3}\times 12l$	$2c$; $(p-1)\times 6i$; $\frac{(p-1)(p-2)}{6}\times 12l$ $p\times 6i$; $\frac{p(p-1)}{2}\times 12l$	$2d$; $(p-1)\times 6j$; $\frac{(p-1)(p-2)}{6}\times 12l$ $p\times 6j$; $\frac{p(p-1)}{2}\times 12l$	$2e$; $(p-1)\times 6k$; $\frac{(p-1)(p-2)}{6}\times 12l$ $p\times 6k$; $\frac{p(p-1)}{2}\times 12l$	$3f$; $\frac{p-1}{2}\times 6i$; $\frac{p-1}{2}\times 6k$; $\frac{(p-1)^2}{4}\times 12l$ $p^2\times 12l$

D_{3d}^2 $P\bar{3}12/c$ No. 163 $P\bar{3}1c$

Subgroup	Axes	Coordinates	$2a$	$2b$	$2c$	$2d$ $6g$	$4e$ $6h$	$4f$ $12i$
I Maximal *translationengleiche* subgroups								
[2] $P31c$ (159)			$2a$	$2a$	$2b$	$2b$ $6c$	$2\times2a$ $6c$	$2\times2b$ $2\times6c$
[2] $P312$ (149)		$x,y,z+\frac{1}{4}$	$1a$; $1b$	$2g$	$1d$; $1e$	$1c$; $1f$ $6l$	$2\times2g$ $3j$; $3k$	$2h$; $2i$ $2\times6l$
[2] $P\bar{3}$ (147)			$2c$	$1a$; $1b$	$2d$	$2d$ $3e$; $3f$	$2\times2c$ $6g$	$2\times2d$ $2\times6g$
[3] $C12/c1$ (15)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y,\frac{1}{2}y,z$	$4e$	$4a$	$4e$	$4e$ $4b$; $4c$; $4d$	$8f$ $4e$; $8f$	$8f$ $3\times8f$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y,-\frac{1}{2}x,z$						
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-(x+y),\frac{1}{2}(x-y),z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[3] $P\bar{3}c1$ (165)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y),z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a$; $4d$	$2b$; $4d$	$6f$	$6f$ $6e$; $12g$	$4c$; $2\times4d$ $6f$; $12g$	$12g$ $3\times12g$
[3] $R\bar{3}c$ (167)	**a**−**b**, **a**+2**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(2x-y),\frac{1}{3}(x+y),\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$6a$; $12c$	$6b$; $12c$	$18e$	$18e$ $18d$; $36f$	$3\times12c$ $18e$; $36f$	$36f$ $3\times36f$
[3] $R\bar{3}c$ (167)	2**a**+**b**, −**a**+**b**, 3**c** (hexagonal axes)	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y),\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$6a$; $12c$	$6b$; $12c$	$18e$	$18e$ $18d$; $36f$	$3\times12c$ $18e$; $36f$	$36f$ $3\times36f$
Enlarged unit cell, isomorphic								
[3] $P\bar{3}1c$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$	$2b$; $4e$	$2d$; $4f$	$2c$; $4f$ $6g$; $12i$	$3\times4e$ $6h$; $12i$	$3\times4f$ $3\times12i$
[p] $P\bar{3}1c$	**a**, **b**, p**c** p = prime > 2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times4e$	$2b$; $\frac{p-1}{2}\times4e$	$2c(d^*)$; $\frac{p-1}{2}\times4f$	$2d(c^*)$; $\frac{p-1}{2}\times4f$ $6g$; $\frac{p-1}{2}\times12i$	$p\times4e$ $6h$; $\frac{p-1}{2}\times12i$	$p\times4f$ $p\times12i$
[4] $P\bar{3}1c$	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6h$	$2b$; $6g$	$2d$; $6h$	$2c$; $6h$ $2\times12i$	$4e$; $12i$ $2\times6h$; $12i$	$4f$; $12i$ $4\times12i$
[p^2] $P\bar{3}1c$	p**a**, p**b**, **c** p = prime > 4;	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12i$	$2b$; $\frac{p^2-1}{6}\times12i$	$2c(d^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12i$	$2d(c^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12i$ $6g$; $\frac{p^2-1}{2}\times12i$	$4e$; $\frac{p^2-1}{3}\times12i$ $p\times6h$; $\frac{p(p-1)}{2}\times12i$	$4f$; $\frac{p^2-1}{3}\times12i$ $p^2\times12i$

* $p=4n-1$ $\quad$ † $p=6n-1$

$P\bar{3}m1$ No. 164 $P\bar{3}2/m1$ D_{3d}^{3}

	Axes	Coordinates	Wyckoff positions					
			$1a$	$1b$	$2c$ $6g$	$2d$ $6h$	$3e$ $6i$	$3f$ $12j$
I Maximal *translationengleiche* subgroups								
[2] $P3m1$ (156)			$1a$	$1a$	$2{\times}1a$ $6e$	$1b; 1c$ $6e$	$3d$ $2{\times}3d$	$3d$ $2{\times}6e$
[2] $P321$ (150)			$1a$	$1b$	$2c$ $2{\times}3e$	$2d$ $2{\times}3f$	$3e$ $6g$	$3f$ $2{\times}6g$
[2] $P\bar{3}$ (147)			$1a$	$1b$	$2c$ $6g$	$2d$ $6g$	$3e$ $6g$	$3f$ $2{\times}6g$
[3] $C12/m1$ (12)	$2\mathbf{a}{+}\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x{+}y, z$	$2a$	$2c$	$4i$ $4g; 8j$	$4i$ $4h; 8j$	$2b; 4e$ $4i; 8j$	$2d; 4f$ $3{\times}8j$
conjugate:	$\mathbf{a}{-}\mathbf{b}, \mathbf{a}{+}\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x{-}y), \frac{1}{2}(x{+}y), z$						
conjugate:	$\mathbf{a}{+}2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x{+}\frac{1}{2}y, z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P\bar{3}c1$ (165)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$2b$	$2a$	$4c$ $12g$	$4d$ $2{\times}6f$	$6e$ $12g$	$6f$ $2{\times}12g$
[2] $P\bar{3}c1$ (165)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z{+}\frac{1}{4}; +(0, 0, \frac{1}{2})$	$2a$	$2b$	$4c$ $2{\times}6f$	$4d$ $12g$	$6f$ $12g$	$6e$ $2{\times}12g$
[3] $P\bar{3}1m$ (162)	$2\mathbf{a}{+}\mathbf{b}, -\mathbf{a}{+}\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x{+}y), \frac{1}{3}(-x{+}2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$1a; 2c$	$1b; 2d$	$2e; 4h$ $3{\times}6i$	$6k$ $3{\times}6j$	$3f; 6i$ $6k; 12l$	$3g; 6j$ $3{\times}12l$
Enlarged unit cell, isomorphic								
[2] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$1a; 1b$	$2c$	$2{\times}2c$ $6g; 6h$	$2{\times}2d$ $12j$	$3e; 3f$ $2{\times}6i$	$6i$ $2{\times}12j$
[2] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z{+}\frac{1}{4}; +(0, 0, \frac{1}{2})$	$2c$	$1a; 1b$	$2{\times}2c$ $12j$	$2{\times}2d$ $6g; 6h$	$6i$ $2{\times}6i$	$3e; 3f$ $2{\times}12j$
[3] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$1a; 2c$	$1b; 2c$	$3{\times}2c$ $6g; 12j$	$3{\times}2d$ $6h; 12j$	$3e; 6i$ $3{\times}6i$	$3f; 6i$ $3{\times}12j$
[p] $P\bar{3}m1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$ $p = \text{prime} > 2; u = 1, \ldots, p-1$	$1a; \frac{p-1}{2}{\times}2c$	$1b; \frac{p-1}{2}{\times}2c$	$p{\times}2c$ $6g; \frac{p-1}{2}{\times}12j$	$p{\times}2d$ $6h; \frac{p-1}{2}{\times}12j$	$3e; \frac{p-1}{2}{\times}6i$ $p{\times}6i$	$3f; \frac{p-1}{2}{\times}6i$ $p{\times}12j$
[4] $P\bar{3}m1$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0); +(0, \frac{1}{2}, 0); +(\frac{1}{2}, \frac{1}{2}, 0)$	$1a; 3e$	$1b; 3f$	$2c; 6i$ $2{\times}6g; 12j$	$2d; 6i$ $2{\times}6h; 12j$	$6g; 6i$ $2{\times}6i; 12j$	$6h; 6i$ $4{\times}12j$
[p^2] $P\bar{3}m1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p = \text{prime} > 4;$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$ $u, v = 1, \ldots, p-1$	$1a; \frac{p-1}{2}{\times}6g;$ $\frac{p-1}{2}{\times}6i;$ $\frac{(p-1)(p-5)}{12}{\times}12j$	$1b; \frac{p-1}{2}{\times}6h;$ $\frac{p-1}{2}{\times}6i;$ $\frac{(p-1)(p-5)}{12}{\times}12j$	$2c;$ $(p-1){\times}6i;$ $\frac{(p-1)(p-2)}{6}{\times}12j$ $p{\times}6g;$ $\frac{p(p-1)}{2}{\times}12j$	$2d;$ $(p-1){\times}6i;$ $\frac{(p-1)(p-2)}{6}{\times}12j$ $p{\times}6h;$ $\frac{p(p-1)}{2}{\times}12j$	$3e; \frac{p-1}{2}{\times}6g;$ $\frac{p-1}{2}{\times}6i;$ $\frac{(p-1)^2}{4}{\times}12j$ $p{\times}6i;$ $\frac{p(p-1)}{2}{\times}12j$	$3f; \frac{p-1}{2}{\times}6h;$ $\frac{p-1}{2}{\times}6i;$ $\frac{(p-1)^2}{4}{\times}12j$ $p^2{\times}12i$

D_{3d}^4 $P\bar{3}2/c1$ No. 165 $P\bar{3}c1$

	Axes	Coordinates	Wyckoff positions						
			$2a$	$2b$	$4c$	$4d$	$6e$	$6f$	$12g$
I Maximal *translationengleiche* subgroups									
[2] $P3c1$ (158)			$2a$	$2a$	$2\times2a$	$2b; 2c$	$6d$	$6d$	$2\times6d$
[2] $P321$ (150)		$x, y, z+\frac{1}{4}$	$1a; 1b$	$2c$	$2\times2c$	$2\times2d$	$6g$	$3e; 3f$	$2\times6g$
[2] $P\bar{3}$ (147)			$2c$	$1a; 1b$	$2\times2c$	$2\times2d$	$3e; 3f$	$6g$	$2\times6g$
[3] $C12/c1$ (15)	2**a**+**b**, **b**, **c**	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	$4e$	$4a$	$8f$	$8f$	$4b; 4c; 4d$	$4e; 8f$	$3\times8f$
conjugate:	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$							
conjugate:	**a**+2**b**, −**a**, **c**	$\frac{1}{2}y, -x+\frac{1}{2}y, z$							
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[3] $P\bar{3}1c$ (163)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{2}{3}, \frac{1}{3}, 0)$	$2a; 2c; 2d$	$2b; 4f$	$4e; 2\times4f$	$12i$	$6g; 12i$	$3\times6h$	$3\times12i$
Enlarged unit cell, isomorphic									
[3] $P\bar{3}c1$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$2a; 4c$	$2b; 4c$	$3\times4c$	$3\times4d$	$6e; 12g$	$6f; 12g$	$3\times12g$
[p] $P\bar{3}c1$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$; $p=$ prime >2; $u=1,\dots,p-1$	$2a; \frac{p-1}{2}\times4c$	$2b; \frac{p-1}{2}\times4c$	$p\times4c$	$p\times4d$	$6e; \frac{p-1}{2}\times12g$	$6f; \frac{p-1}{2}\times12g$	$p\times12g$
[4] $P\bar{3}c1$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0); +(0, \frac{1}{2}, 0); +(\frac{1}{2}, \frac{1}{2}, 0)$	$2a; 6f$	$2b; 6e$	$4c; 12g$	$4d; 12g$	$2\times12g$	$2\times6f; 12g$	$4\times12g$
[p^2] $P\bar{3}c1$	p**a**, p**b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$; $p=$ prime >4; $u, v=1,\dots,p-1$	$2a; (p-1)\times6f; \frac{(p-1)(p-2)}{6}\times12g$	$2b; \frac{p^2-1}{6}\times12g$	$4c; \frac{p^2-1}{3}\times12g$	$4d; \frac{p^2-1}{3}\times12g$	$6e; \frac{p^2-1}{2}\times12g$	$p\times6f; \frac{p(p-1)}{2}\times12g$	$p^2\times12g$

$R\bar{3}m$ No. 166 $R\bar{3}2/m$ D_{3d}^{5}

HEXAGONAL AXES

	Axes	Coordinates	Wyckoff positions $3a$	 $3b$ $18f$	 $6c$ $18g$	 $9d$ $18h$	 $9e$ $36i$
I Maximal *translationengleiche* subgroups							
[2] $R3m$ (160)			$3a$	$3a$ $18c$	$2\times3a$ $18c$	$9b$ $2\times9b$	$9b$ $2\times18c$
[2] $R32$ (155)			$3a$	$3b$ $2\times9d$	$6c$ $2\times9e$	$9e$ $18f$	$9d$ $2\times18f$
[2] $R\bar{3}$ (148)			$3a$	$3b$ $18f$	$6c$ $18f$	$9d$ $18f$	$9e$ $2\times18f$
[3] $C12/m1$ (12)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c}), \mathbf{b}, \frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}x-z, -\frac{1}{2}x+y, x+z$	$2a$	$2d$ $4g; 8j$	$4i$ $4h; 8j$	$2c; 4e$ $4i; 8j$	$2b; 4f$ $3\times8j$
conjugate:	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \frac{1}{3}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$	$-\frac{1}{2}x+\frac{1}{2}y-z, -\frac{1}{2}x-\frac{1}{2}y, -x+y+z$					
conjugate:	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$	$-\frac{1}{2}y-z, x-\frac{1}{2}y, -y+z$					
alternative:	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c}), \mathbf{b}, \mathbf{c}$	$\frac{3}{2}x, -\frac{1}{2}x+y, x+z$	$2a$	$2c$ $4g; 8j$	$4i$ $4h; 8j$	$2d; 4e$ $4i; 8j$	$2b; 4f$ $3\times8j$
or	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c}), -\mathbf{a}-\mathbf{b}, \mathbf{c}$	$\frac{3}{2}(-x+y), -\frac{1}{2}(x+y), -x+y+z$					
or	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c}), \mathbf{a}, \mathbf{c}$	$-\frac{3}{2}y, x-\frac{1}{2}y, -y+z$					
alternative:	$2\mathbf{a}+\mathbf{b}, -\mathbf{b}, -\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}x-z, \frac{1}{2}x-y, -3z$	$2a$	$2d$ $4g; 8j$	$4i$ $4h; 8j$	$2c; 4f$ $4i; 8j$	$2b; 4e$ $3\times8j$
or	$-\mathbf{a}+\mathbf{b}, \mathbf{a}+\mathbf{b}, \frac{1}{3}(\mathbf{a}-\mathbf{b}-\mathbf{c})$	$\frac{1}{2}(-x+y)-z, \frac{1}{2}(x+y), -3z$					
or	$-\mathbf{a}-2\mathbf{b}, -\mathbf{a}, \frac{1}{3}(\mathbf{a}+2\mathbf{b}-\mathbf{c})$	$-\frac{1}{2}y-z, -x+\frac{1}{2}y, -3z$					
II Maximal *klassengleiche* subgroups							
Loss of centring translations							
[3] $P\bar{3}m1$ (164)	3 conjugate subgroups		$1a; 2d$	$1b; 2d$ $6g; 12j$	$2c; 2\times2d$ $6h; 12j$	$3f; 6i$ $3\times6i$	$3e; 6i$ $3\times12j$
Enlarged unit cell, non-isomorphic							
[2] $R\bar{3}c$ (167)	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$6b$	$6a$ $36f$	$12c$ $2\times18e$	$18e$ $36f$	$18d$ $2\times36f$
[2] $R\bar{3}c$ (167)	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$6a$	$6b$ $2\times18e$	$12c$ $36f$	$18d$ $36f$	$18e$ $2\times36f$
Enlarged unit cell, isomorphic							
[2] $R\bar{3}m$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$3a; 3b$	$6c$ $18f; 18g$	$2\times6c$ $36i$	$18h$ $2\times18h$	$9d; 9e$ $2\times36i$
[2] $R\bar{3}m$	$-\mathbf{a}, -\mathbf{b}, 2\mathbf{c}$	$-x, -y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$6c$	$3a; 3b$ $36i$	$2\times6c$ $18f; 18g$	$9d; 9e$ $2\times18h$	$18h$ $2\times36i$
[p] $R\bar{3}m$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$ $p=\text{prime}=6n-1; u=1,\ldots,p-1$	$-x, -y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$3a; \frac{p-1}{2}\times6c$	$3b; \frac{p-1}{2}\times6c$ $18f; \frac{p-1}{2}\times36i$	$p\times6c$ $18g; \frac{p-1}{2}\times36i$	$9d; \frac{p-1}{2}\times18h$ $p\times18h$	$9e; \frac{p-1}{2}\times18h$ $p\times36i$
	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p=\text{prime}=6n+1; u=1,\ldots,p-1$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$					
[4] $R\bar{3}m$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$3a; 9e$	$3b; 9d$ $2\times18f; 36i$	$6c; 18h$ $2\times18g; 36i$	$18g; 18h$ $2\times18h; 36i$	$18f; 18h$ $4\times36i$
[p^2] $R\bar{3}m$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$ $p=\text{prime}=6n-1; u,v=1,\ldots,p-1$	$-\frac{1}{p}x, -\frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$3a; \frac{p-1}{2}\times18f$; $\frac{p-1}{2}\times18h$; $\frac{(p-1)(p-5)}{12}\times36i$	$3b; \frac{p-1}{2}\times18g$; $\frac{p-1}{2}\times18h$; $\frac{(p-1)(p-5)}{12}\times36i$	$6c$; $(p-1)\times18h$; $\frac{(p-1)(p-2)}{6}\times36i$	$9d; \frac{p-1}{2}\times18g$; $\frac{p-1}{2}\times18h$; $\frac{(p-1)^2}{4}\times36i$	$9e; \frac{p-1}{2}\times18f$; $\frac{p-1}{2}\times18h$; $\frac{(p-1)^2}{4}\times36i$
	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p=\text{prime}=6n+1; u,v=1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$		$p\times18f$; $\frac{p(p-1)}{2}\times36i$	$p\times18g$; $\frac{p(p-1)}{2}\times36i$	$p\times18h$; $\frac{p(p-1)}{2}\times36i$	$p^2\times36i$

D_{3d}^{6} $\quad R\bar{3}2/c$ $\quad$ No. 167 $\quad R\bar{3}c$

HEXAGONAL AXES

	Axes	Coordinates	Wyckoff positions 6*a*	6*b*	12*c*	18*d*	18*e*	36*f*
I Maximal *translationengleiche* subgroups								
[2] $R3c$ (161)			6*a*	6*a*	2×6*a*	18*b*	18*b*	2×18*b*
[2] $R32$ (155)		$x, y, z+\frac{1}{4}$	3*a*; 3*b*	6*c*	2×6*c*	18*f*	9*d*; 9*e*	2×18*f*
[2] $R\bar{3}$ (148)			6*c*	3*a*; 3*b*	2×6*c*	9*d*; 9*e*	18*f*	2×18*f*
[3] $C12/c1$ (15)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}-2\mathbf{c})$, $\mathbf{b}$, $\mathbf{c}$	$\frac{2}{3}x, -\frac{1}{2}x+y, x+z$	4*e*	4*a*	8*f*	4*b*; 4*c*; 4*d*	4*e*; 8*f*	3×18*f*
conjugate:	$\frac{1}{3}(-\mathbf{a}+\mathbf{b}-2\mathbf{c})$, $-\mathbf{a}-\mathbf{b}$, $\mathbf{c}$	$\frac{3}{2}(-x+y), \frac{1}{2}(-x-y), -x+y+z$						
conjugate:	$\frac{1}{3}(-\mathbf{a}-2\mathbf{b}-2\mathbf{c})$, $\mathbf{a}$, $\mathbf{c}$	$-\frac{3}{2}y, x-\frac{1}{2}y, -y+z$						
alternative:	$2\mathbf{a}+\mathbf{b}$, $\mathbf{b}$, $-\frac{2}{3}(2\mathbf{a}+\mathbf{b})+\frac{1}{3}\mathbf{c}$	$\frac{1}{2}x+2z, -\frac{1}{2}x+y, 3z$						
or	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{a}-\mathbf{b}$, $\frac{2}{3}(\mathbf{a}-\mathbf{b})+\frac{1}{3}\mathbf{c}$	$\frac{1}{2}(-x+y)+2z, -\frac{1}{2}(x+y), 3z$						
or	$-\mathbf{a}-2\mathbf{b}$, $\mathbf{a}$, $\frac{2}{3}(\mathbf{a}+2\mathbf{b})+\frac{1}{3}\mathbf{c}$	$-\frac{1}{2}y+2z, x-\frac{1}{2}y, 3z$						
Loss of centring translations								
[3] $P\bar{3}c1$ (165)	3 conjugate subgroups		2*a*; 4*d*	2*b*; 4*d*	4*c*; 2×4*d*	6*e*; 12*g*	6*f*; 12*g*	3×12*g*
Enlarged unit cell, isomorphic								
[5] $R\bar{3}c$	$-\mathbf{a}, -\mathbf{b}, 5\mathbf{c}$	$-x, -y, \frac{1}{5}z$; $\pm(0,0,\frac{1}{5})$; $\pm(0,0,\frac{2}{5})$	6*a*; 2×12*c*	6*b*; 2×12*c*	5×12*c*	18*d*; 2×36*f*	18*e*; 2×36*f*	5×36*f*
[p] $R\bar{3}c$	$-\mathbf{a}, -\mathbf{b}, p\mathbf{c}$; p = prime = $6n-1$; $u = 1, \ldots, p-1$	$-x, -y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	6*a*; $\frac{p-1}{2}\times 12c$	6*b*; $\frac{p-1}{2}\times 12c$	$p\times 12c$	18*d*; $\frac{p-1}{2}\times 36f$	18*e*; $\frac{p-1}{2}\times 36f$	$p\times 36f$
	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$; p = prime = $6n+1$; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$						
[4] $R\bar{3}c$	$-2\mathbf{a}, -2\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x, -\frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	6*a*; 18*e*	6*b*; 18*d*	12*c*; 36*f*	2×36*f*	2×18*e*; 36*f*	4×36*f*
[p^2] $R\bar{3}c$	$-p\mathbf{a}, -p\mathbf{b}, \mathbf{c}$; p = prime = $6n-1$; $u, v = 1, \ldots, p-1$	$-\frac{1}{p}x, -\frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	6*a*; $(p-1)\times 18e$; $\frac{(p-1)(p-2)}{6}\times 36f$	6*b*; $\frac{p^2-1}{6}\times 36f$	12*c*; $\frac{p^2-1}{3}\times 36f$	18*d*; $\frac{p^2-1}{2}\times 36f$	$p\times 18e$; $\frac{p(p-1)}{2}\times 36f$	$p^2\times 36f$
	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$; p = prime = $6n+1$; $u, v = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$						

$P6$ No. 168 C_6^1

Axes	Coordinates		Wyckoff positions			
			$1a$	$2b$	$3c$	$6d$
I Maximal *translationengleiche* subgroups						
[2] $P3$ (143)			$1a$	$1b; 1c$	$3d$	$2\times3d$
[3] $P112$ (3)			$1a$	$2e$	$1b; 1c; 1d$	$3\times2e$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[2] $P6_3$ (173)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$2a$	$2\times2b$	$6c$	$2\times6c$
[3] $P6_4$ (172)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3a$	$6c$	$3\times3b$	$3\times6c$
[3] $P6_2$ (171)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3a$	$6c$	$3\times3b$	$3\times6c$
Enlarged unit cell, isomorphic						
[2] $P6$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0, 0, \frac{1}{2})$	$2\times1a$	$2\times2b$	$2\times3c$	$2\times6d$
[3] $P6$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0, 0, \frac{1}{3})$	$3\times1a$	$3\times2b$	$3\times3c$	$3\times6d$
[p] $P6$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime; $u = 1, \ldots, p-1$	$x, y, \frac{1}{p}z; +(0, 0, \frac{u}{p})$	$p\times1a$	$p\times2b$	$p\times3c$	$p\times6d$
[3] $P6$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3}, \frac{2}{3}, 0)$	$1a; 2b$	$6d$	$3c; 6d$	$3\times6d$
[7] $P6$	$3\mathbf{a}+\mathbf{b}, -\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z; \pm(\frac{1}{7}, \frac{3}{7}, 0);$ $\pm(\frac{3}{7}, \frac{2}{7}, 0); \pm(\frac{5}{7}, \frac{1}{7}, 0)$	$1a; 6d$	$2b; 2\times6d$	$3c; 3\times6d$	$7\times6d$
[7] $P6$	$3\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z; \pm(\frac{2}{7}, \frac{3}{7}, 0);$ $\pm(\frac{3}{7}, \frac{1}{7}, 0); \pm(\frac{1}{7}, \frac{5}{7}, 0)$	$1a; 6d$	$2b; 2\times6d$	$3c; 3\times6d$	$7\times6d$
[p] $P6$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$ p = prime = $q^2-qr+r^2 = 6n+1$; $q, r = 1, 2, \ldots; q > r; u = 1, \ldots, p-1$	$\frac{1}{p}((q-r)x+ry), \frac{1}{p}(-rx+qy), z;$ $+(\frac{ur}{p}, \frac{uq}{p}, 0)$	$1a; \frac{p-1}{6}\times6d$	$2b; \frac{p-1}{3}\times6d$	$3c; \frac{p-1}{2}\times6d$	$p\times6d$
[4] $P6$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2}, 0, 0); +(0, \frac{1}{2}, 0); +(\frac{1}{2}, \frac{1}{2}, 0)$	$1a; 3c$	$2b; 6d$	$2\times6d$	$4\times6d$
[p^2] $P6$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime = $6n-1$; $u, v = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p}, \frac{v}{p}, 0)$	$1a; \frac{p^2-1}{6}\times6d$	$2b; \frac{p^2-1}{3}\times6d$	$3c; \frac{p^2-1}{2}\times6d$	$p^2\times6d$

$P6_1$ No. 169 C_6^2 C_6^3 No. 170 $P6_5$

	Axes	Coordinates	Wyckoff Positions		Axes	Coordinates
			$6a$			
I Maximal *translationengleiche* subgroups						
[2] $P3_1$ (144)			$2\times3a$	[2] $P3_2$ (145)		
[3] $P112_1$ (4)			$3\times2a$	[3] $P112_1$ (4)		
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[5] $P6_5$ (170)	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$	$5\times6a$	[5] $P6_1$ (169)	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x, y, \frac{1}{5}z; \pm(0,0,\frac{1}{5}); \pm(0,0,\frac{2}{5})$
[p] $P6_5$ (170)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime $= 6n-1$; $u = 1,\ldots,p-1$	$p\times6a$	[p] $P6_1$ (169)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime $= 6n-1$; $u = 1,\ldots,p-1$
[7] $P6_1$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z; \pm(0,0,\frac{1}{7})$; $\pm(0,0,\frac{2}{7}); \pm(0,0,\frac{3}{7})$	$7\times6a$	[7] $P6_5$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x, y, \frac{1}{7}z; \pm(0,0,\frac{1}{7})$; $\pm(0,0,\frac{2}{7}); \pm(0,0,\frac{3}{7})$
[p] $P6_1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime $= 6n+1$; $u = 1,\ldots,p-1$	$p\times6a$	[p] $P6_5$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$ p = prime $= 6n+1$; $u = 1,\ldots,p-1$
[3] $P6_1$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3},\frac{2}{3},0)$	$3\times6a$	[3] $P6_5$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3},\frac{2}{3},0)$
[7] $P6_1$	$3\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z$; $\pm(\frac{1}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{2}{7},0); \pm(\frac{5}{7},\frac{1}{7},0)$	$7\times6a$	[7] $P6_5$	$3\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z$; $\pm(\frac{1}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{2}{7},0); \pm(\frac{5}{7},\frac{1}{7},0)$
[7] $P6_1$	$3\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z$; $\pm(\frac{2}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{1}{7},0); \pm(\frac{1}{7},\frac{5}{7},0)$	$7\times6a$	[7] $P6_5$	$3\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z$; $\pm(\frac{2}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{1}{7},0); \pm(\frac{1}{7},\frac{5}{7},0)$
[p] $P6_1$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$	$\frac{1}{p}((q-r)x+ry), \frac{1}{p}(-rx+qy), z$; $+(\frac{ur}{p},\frac{uq}{p},0)$ p = prime $= q^2-qr+r^2 = 6n+1$; $q,r = 1,2,\ldots;\ q > r;\ u = 1,\ldots,p-1$	$p\times6a$	[p] $P6_5$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$	$\frac{1}{p}((q-r)x+ry), \frac{1}{p}(-rx+qy), z$; $+(\frac{ur}{p},\frac{uq}{p},0)$ p = prime $= q^2-qr+r^2 = 6n+1$; $q,r = 1,2,\ldots;\ q > r;\ u = 1,\ldots,p-1$
[4] $P6_1$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$4\times6a$	[4] $P6_5$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$
[p^2] $P6_1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$ p = prime $= 3n-1$; $u,v = 1,\ldots,p-1$	$p^2\times6a$	[p^2] $P6_5$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$ p = prime $= 3n-1$; $u,v = 1,\ldots,p-1$

$P6_2$ No. 171 C_6^4 — $P6_4$ No. 172 C_6^5

$P6_2$ (171)	Axes	Coordinates	Wyckoff positions $3a$	$3b$	$6c$	$P6_4$ (172)	Axes	Coordinates
I Maximal *translationengleiche* subgroups								
[2] $P3_2$ (145)			$3a$	$3a$	$3{\times}3a$	[2] $P3_1$ (144)		
[3] $P112$ (3)			$3{\times}1a$	$1b;1c;1d$	$3{\times}2e$	[3] $P112$ (3)		
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P6_1$ (169)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$6a$	$6a$	$2{\times}6a$	[2] $P6_5$ (170)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$
Enlarged unit cell, isomorphic								
[2] $P6_4$ (172)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2{\times}3a$	$2{\times}3b$	$2{\times}6c$	[2] $P6_2$ (171)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$
[5] $P6_4$ (172)	$\mathbf{a},\mathbf{b},5\mathbf{c}$	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});\ \pm(0,0,\frac{2}{5})$	$5{\times}3a$	$5{\times}3b$	$5{\times}6c$	[5] $P6_2$ (171)	$\mathbf{a},\mathbf{b},5\mathbf{c}$	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});\ \pm(0,0,\frac{2}{5})$
[p] $P6_4$ (172)	$\mathbf{a},\mathbf{b},p\mathbf{c}$; p = prime = $3n-1$; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p{\times}3a$	$p{\times}3b$	$p{\times}6c$	[p] $P6_2$ (171)	$\mathbf{a},\mathbf{b},p\mathbf{c}$; p = prime = $3n-1$; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$
[7] $P6_2$	$\mathbf{a},\mathbf{b},7\mathbf{c}$	$x,y,\frac{1}{7}z;\ \pm(0,0,\frac{1}{7});\ \pm(0,0,\frac{2}{7});\ \pm(0,0,\frac{3}{7})$	$7{\times}3a$	$7{\times}3b$	$7{\times}6c$	[7] $P6_4$	$\mathbf{a},\mathbf{b},7\mathbf{c}$	$x,y,\frac{1}{7}z;\ \pm(0,0,\frac{1}{7});\ \pm(0,0,\frac{2}{7});\ \pm(0,0,\frac{3}{7})$
[p] $P6_2$	$\mathbf{a},\mathbf{b},p\mathbf{c}$; p = prime = $6n+1$; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p{\times}3a$	$p{\times}3b$	$p{\times}6c$	[p] $P6_4$	$\mathbf{a},\mathbf{b},p\mathbf{c}$; p = prime = $6n+1$; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$
[3] $P6_2$	$2\mathbf{a}+\mathbf{b},\ -\mathbf{a}+\mathbf{b},\ \mathbf{c}$	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y),z;\ \pm(\frac{1}{3},\frac{2}{3},0)$	$3a;6c$	$3b;6c$	$3{\times}6c$	[3] $P6_4$	$2\mathbf{a}+\mathbf{b},\ -\mathbf{a}+\mathbf{b},\ \mathbf{c}$	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y),z;\ \pm(\frac{1}{3},\frac{2}{3},0)$
[7] $P6_2$	$3\mathbf{a}+\mathbf{b},\ -\mathbf{a}+2\mathbf{b},\ \mathbf{c}$	$\frac{1}{7}(2x+y),\frac{1}{7}(-x+3y),z;\ \pm(\frac{1}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{2}{7},0);\ \pm(\frac{5}{7},\frac{1}{7},0)$	$3a;3{\times}6c$	$3b;3{\times}6c$	$7{\times}6c$	[7] $P6_4$	$3\mathbf{a}+\mathbf{b},\ -\mathbf{a}+2\mathbf{b},\ \mathbf{c}$	$\frac{1}{7}(2x+y),\frac{1}{7}(-x+3y),z;\ \pm(\frac{1}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{2}{7},0);\ \pm(\frac{5}{7},\frac{1}{7},0)$
[7] $P6_2$	$3\mathbf{a}+2\mathbf{b},\ -2\mathbf{a}+\mathbf{b},\ \mathbf{c}$	$\frac{1}{7}(x+2y),\frac{1}{7}(-2x+3y),z;\ \pm(\frac{2}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{1}{7},0);\ \pm(\frac{1}{7},\frac{5}{7},0)$	$3a;3{\times}6c$	$3b;3{\times}6c$	$7{\times}6c$	[7] $P6_4$	$3\mathbf{a}+2\mathbf{b},\ -2\mathbf{a}+\mathbf{b},\ \mathbf{c}$	$\frac{1}{7}(x+2y),\frac{1}{7}(-2x+3y),z;\ \pm(\frac{2}{7},\frac{3}{7},0);\ \pm(\frac{3}{7},\frac{1}{7},0);\ \pm(\frac{1}{7},\frac{5}{7},0)$
[p] $P6_2$	$q\mathbf{a}+r\mathbf{b},\ -r\mathbf{a}+(q-r)\mathbf{b},\ \mathbf{c}$; p = prime = $q^2-qr+r^2=6n+1$; $q,r=1,2,\dots;\ q>r;\ u=1,\dots,p-1$	$\frac{1}{p}((q-r)x+ry),\ \frac{1}{p}(-rx+qy),z;+(\frac{ur}{p},\frac{uq}{p},0)$	$3a;\frac{p-1}{2}{\times}6c$	$3b;\frac{p-1}{2}{\times}6c$	$p{\times}6c$	[p] $P6_4$	$q\mathbf{a}+r\mathbf{b},\ -r\mathbf{a}+(q-r)\mathbf{b},\ \mathbf{c}$; p = prime = $q^2-qr+r^2=6n+1$; $q,r=1,2,\dots;\ q>r;\ u=1,\dots,p-1$	$\frac{1}{p}((q-r)x+ry),\ \frac{1}{p}(-rx+qy),z;+(\frac{ur}{p},\frac{uq}{p},0)$
[4] $P6_2$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z;\ +(\frac{1}{2},0,0);\ +(0,\frac{1}{2},0);\ +(\frac{1}{2},\frac{1}{2},0)$	$3a;3{\times}3b$	$2{\times}6c$	$4{\times}6c$	[4] $P6_4$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z;\ +(\frac{1}{2},0,0);\ +(0,\frac{1}{2},0);\ +(\frac{1}{2},\frac{1}{2},0)$
[p^2] $P6_2$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$; p = prime = $6n-1$; $u,v=1,\dots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$3a;\frac{p^2-1}{2}{\times}6c$	$3b;\frac{p^2-1}{2}{\times}6c$	$p^2{\times}6c$	[p^2] $P6_4$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$; p = prime = $6n-1$; $u,v=1,\dots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$

C_6^6 No. 173 $P6_3$

	Axes	Coordinates	2a	2b	6c
I Maximal *translationengleiche* subgroups					
[2] $P3$ (143)			$2\times1a$	$1b$; $1c$	$2\times3d$
[3] $P112_1$ (4)			$2a$	$2a$	$3\times2a$
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, non-isomorphic					
[3] $P6_5$ (170)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$6a$	$6a$	$3\times6a$
[3] $P6_1$ (169)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$6a$	$6a$	$3\times6a$
Enlarged unit cell, isomorphic					
[3] $P6_3$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times6c$
[p] $P6_3$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$p\times2a$	$p\times2b$	$p\times6c$
	p = prime > 2; $u = 1,\ldots,p-1$				
[3] $P6_3$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a$; $2\times2b$	$6c$	$3\times6c$
[7] $P6_3$	$3\mathbf{a}+\mathbf{b}, -\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z$; $\pm(\frac{1}{7},\frac{3}{7},0)$; $\pm(\frac{3}{7},\frac{2}{7},0)$; $\pm(\frac{5}{7},\frac{1}{7},0)$	$2a$; $2\times6c$	$2b$; $2\times6c$	$7\times6c$
[7] $P6_3$	$3\mathbf{a}+2\mathbf{b}, -2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z$; $\pm(\frac{2}{7},\frac{3}{7},0)$; $\pm(\frac{3}{7},\frac{1}{7},0)$; $\pm(\frac{1}{7},\frac{5}{7},0)$	$2a$; $2\times6c$	$2b$; $2\times6c$	$7\times6c$
[p] $P6_3$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$	$\frac{1}{p}((q-r)x+ry), \frac{1}{p}(-rx+qy), z$; $+(\frac{ur}{p},\frac{uq}{p},0)$	$2a$; $\frac{p-1}{3}\times6c$	$2b$; $\frac{p-1}{3}\times6c$	$p\times6c$
	p = prime $= q^2-qr+r^2 = 6n+1$; $q, r = 1,2,\ldots$; $q > r$; $u = 1,\ldots,p-1$				
[4] $P6_3$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6c$	$2b$; $6c$	$4\times6c$
[p^2] $P6_3$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a$; $\frac{p^2-1}{3}\times6c$	$2b$; $\frac{p^2-1}{3}\times6c$	$p^2\times6c$
	p = prime $= 3n-1$; $u, v = 1,\ldots,p-1$				

$P\bar{6}$ No. 174 C_{3h}^1

	Axes	Coordinates	Wyckoff positions						
			$1a$	$1b$	$1c$ $2h$	$1d$ $2i$	$1e$ $3j$	$1f$ $3k$	$2g$ $6l$
I Maximal *translationengleiche* subgroups									
[2] $P3$ (143)			$1a$	$1a$	$1b$ $2\times 1b$	$1b$ $2\times 1c$	$1c$ $3d$	$1c$ $3d$	$2\times 1a$ $2\times 3d$
[3] $P11m$ (6)			$1a$	$1b$	$1a$ $2c$	$1b$ $2c$	$1a$ $3\times 1a$	$1b$ $3\times 1b$	$2c$ $3\times 2c$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**									
[2] $P\bar{6}$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$1a; 1b$	$2g$	$1c; 1d$ $2\times 2h$	$2h$ $2\times 2i$	$1e; 1f$ $3j; 3k$	$2i$ $6l$	$2\times 2g$ $2\times 6l$
[2] $P\bar{6}$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$2g$	$1a; 1b$	$2h$ $2\times 2h$	$1c; 1d$ $2\times 2i$	$2i$ $6l$	$1e; 1f$ $3j; 3k$	$2\times 2g$ $2\times 6l$
[3] $P\bar{6}$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$1a; 2g$	$1b; 2g$	$1c; 2h$ $3\times 2h$	$1d; 2h$ $3\times 2i$	$1e; 2i$ $3j; 6l$	$1f; 2i$ $3k; 6l$	$3\times 2g$ $3\times 6l$
[p] $P\bar{6}$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$ p = prime > 2; $u = 1,\ldots,p-1$	$1a;$ $\frac{p-1}{2}\times 2g$	$1b;$ $\frac{p-1}{2}\times 2g$	$1c;$ $\frac{p-1}{2}\times 2h$ $p\times 2h$	$1d;$ $\frac{p-1}{2}\times 2h$ $p\times 2i$	$1e;$ $\frac{p-1}{2}\times 2i$ $3j;$ $\frac{p-1}{2}\times 6l$	$1f;$ $\frac{p-1}{2}\times 2i$ $3k;$ $\frac{p-1}{2}\times 6l$	$p\times 2g$ $p\times 6l$
[3] $P\bar{6}$	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a; 1c; 1e$	$1b; 1d; 1f$	$3j$ $6l$	$3k$ $6l$	$3j$ $3\times 3j$	$3k$ $3\times 3k$	$2g; 2h; 2i$ $3\times 6l$
[3] $P\bar{6}$	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$3j$	$3k$	$1a; 1c; 1e$ $2g; 2h; 2i$	$1b; 1d; 1f$ $6l$	$3j$ $3\times 3j$	$3k$ $3\times 3k$	$6l$ $3\times 6l$
[3] $P\bar{6}$	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$3j$	$3k$	$3j$ $6l$	$3k$ $2g; 2h; 2i$	$1a; 1c; 1e$ $3\times 3j$	$1b; 1d; 1f$ $3\times 3k$	$6l$ $3\times 6l$
[7] $P\bar{6}$	3**a**+**b**, −**a**+2**b**, **c**	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z;$ $\pm(\frac{1}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{2}{7},0); \pm(\frac{5}{7},\frac{1}{7},0)$	$1a; 2\times 3j$	$1b; 2\times 3k$	$1c; 2\times 3j$ $2h; 2\times 6l$	$1d; 2\times 3k$ $2i; 2\times 6l$	$1e; 2\times 3j$ $p\times 3j$	$1f; 2\times 3k$ $p\times 3k$	$2g; 2\times 6l$ $p\times 6l$
[7] $P\bar{6}$	3**a**+2**b**, −2**a**+**b**, **c**	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z;$ $\pm(\frac{2}{7},\frac{3}{7},0); \pm(\frac{3}{7},\frac{1}{7},0); \pm(\frac{1}{7},\frac{5}{7},0)$	$1a; 2\times 3j$	$1b; 2\times 3k$	$1e; 2\times 3j$ $2i; 2\times 6l$	$1f; 2\times 3k$ $2h; 2\times 6l$	$1c; 2\times 3j$ $p\times 3j$	$1d; 2\times 3k$ $p\times 3k$	$2g; 2\times 6l$ $p\times 6l$
[p] $P\bar{6}$	q**a**+r**b**, −r**a**+(q−r)**b**, **c**	$\frac{1}{p}((q-r)x+ry),$ $\frac{1}{p}(-rx+qy), z; +(\frac{ur}{p},\frac{uq}{p},0)$ p = prime $= q^2-qr+r^2 = 6n+1$; $q, r = 1,2,\ldots;\ q > r;\ u = 1,\ldots,p-1$	$1a;$ $\frac{p-1}{3}\times 3j$	$1b;$ $\frac{p-1}{3}\times 3k$	$1c(e^*);$ $\frac{p-1}{3}\times 3j$ $2h(i^*);$ $\frac{p-1}{3}\times 6l$	$1d(f^*);$ $\frac{p-1}{3}\times 3k$ $2i(h^*);$ $\frac{p-1}{3}\times 6l$	$1e(c^*);$ $\frac{p-1}{3}\times 3j$ $p\times 3j$	$1f(d^*);$ $\frac{p-1}{3}\times 3k$ $p\times 3k$	$2g;$ $\frac{p-1}{3}\times 6l$ $p\times 6l$
[4] $P\bar{6}$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$1a; 3j$	$1b; 3k$	$1e; 3j$ $2i; 6l$	$1f; 3k$ $2h; 6l$	$1c; 3j$ $4\times 3j$	$1d; 3k$ $4\times 3k$	$2g; 6l$ $4\times 6l$
[p^2] $P\bar{6}$	p**a**, p**b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$ p = prime $= 3n-1$; $u, v = 1,\ldots,p-1$	$1a;$ $\frac{p^2-1}{3}\times 3j$	$1b;$ $\frac{p^2-1}{3}\times 3k$	$1e;$ $\frac{p^2-1}{3}\times 3j$ $2i;$ $\frac{p^2-1}{3}\times 6l$	$1f;$ $\frac{p^2-1}{3}\times 3k$ $2h;$ $\frac{p^2-1}{3}\times 6l$	$1c;$ $\frac{p^2-1}{3}\times 3j$ $p^2\times 3j$	$1d;$ $\frac{p^2-1}{3}\times 3k$ $p^2\times 3k$	$2g;$ $\frac{p^2-1}{3}\times 6l$ $p^2\times 6l$

$^*\ q+r = 3n-1$

C^1_{6h} No. 175 $P6/m$

	Axes	Coordinates	$1a$	$1b$	$2c$ $4h$	$2d$ $6i$	$2e$ $6j$	$3f$ $6k$	$3g$ $12l$
I Maximal *translationengleiche* subgroups									
[2] $P\bar{6}$ (174)			$1a$	$1b$	$1c;1e$ $2h;2i$	$1d;1f$ $6l$	$2g$ $2\times3j$	$3j$ $2\times3k$	$3k$ $2\times6l$
[2] $P6$ (168)			$1a$	$1a$	$2b$ $2\times2b$	$2b$ $2\times3c$	$2\times1a$ $6d$	$3c$ $6d$	$3c$ $2\times6d$
[2] $P\bar{3}$ (147)			$1a$	$1b$	$2d$ $2\times2d$	$2d$ $6g$	$2c$ $6g$	$3e$ $6g$	$3f$ $2\times6g$
[3] $P112/m$ (10)			$1a$	$1b$	$2m$ $4o$	$2n$ $2j;2k;2l$	$2i$ $3\times2m$	$1c;1d;1g$ $3\times2n$	$1e;1f;1h$ $3\times4o$
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $P6_3/m$ (176)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2b$	$2a$	$4f$ $2\times4f$	$2c;2d$ $12i$	$4e$ $12i$	$6g$ $2\times6h$	$6h$ $2\times12i$
[2] $P6_3/m$ (176)	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$2a$	$2b$	$2c;2d$ $2\times4f$	$4f$ $12i$	$4e$ $2\times6h$	$6h$ $12i$	$6g$ $2\times12i$
Enlarged unit cell, isomorphic									
[2] $P6/m$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$1a;1b$	$2e$	$2c;2d$ $2\times4h$	$4h$ $2\times6i$	$2\times2e$ $6j;6k$	$3f;3g$ $12l$	$6i$ $2\times12l$
[2] $P6/m$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};\ +(0,0,\frac{1}{2})$	$2e$	$1a;1b$	$4h$ $2\times4h$	$2c;2d$ $2\times6i$	$2\times2e$ $12l$	$6i$ $6j;6k$	$3f;3g$ $2\times12l$
[3] $P6/m$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$1a;2e$	$1b;2e$	$2c;4h$ $3\times4h$	$2d;4h$ $3\times6i$	$3\times2e$ $6j;12l$	$3f;6i$ $6k;12l$	$3g;6i$ $3\times12l$
[p] $P6/m$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=$ prime >2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$1a;$ $\frac{p-1}{2}\times2e$	$1b;$ $\frac{p-1}{2}\times2e$	$2c;$ $\frac{p-1}{2}\times4h$ $p\times4h$	$2d;$ $\frac{p-1}{2}\times4h$ $p\times6i$	$p\times2e$ $6j;$ $\frac{p-1}{2}\times12l$	$3f;$ $\frac{p-1}{2}\times6i$ $6k;$ $\frac{p-1}{2}\times6l$	$3g;$ $\frac{p-1}{2}\times6i$ $p\times12l$
[3] $P6/m$	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y),z;$ $\pm(\frac{2}{3},\frac{1}{3},0)$	$1a;2c$	$1b;2d$	$6j$ $12l$	$6k$ $6i;12l$	$2e;4h$ $3\times6j$	$3f;6j$ $3\times6k$	$3g;6k$ $3\times12l$
[7] $P6/m$	$3\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+2\mathbf{b},\mathbf{c}$	$\frac{1}{7}(2x+y),\frac{1}{7}(-x+3y),z;$ $\pm(\frac{1}{7},\frac{3}{7},0);\pm(\frac{3}{7},\frac{2}{7},0);\pm(\frac{5}{7},\frac{1}{7},0)$	$1a;6j$	$1b;6k$	$2c;2\times6j$ $4h;2\times12l$	$2d;2\times6k$ $6i;3\times12l$	$2e;12l$ $7\times6j$	$3f;3\times6j$ $7\times6k$	$3g;3\times6k$ $7\times12l$
[7] $P6/m$	$3\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b},\mathbf{c}$	$\frac{1}{7}(x+2y),\frac{1}{7}(-2x+3y),z;$ $\pm(\frac{2}{7},\frac{3}{7},0);\pm(\frac{3}{7},\frac{1}{7},0);\pm(\frac{1}{7},\frac{5}{7},0)$	$1a;6j$	$1b;6k$	$2c;2\times6j$ $4h;2\times12l$	$2d;2\times6k$ $6i;3\times12l$	$2e;12l$ $7\times6j$	$3f;3\times6j$ $7\times6k$	$3g;3\times6k$ $7\times12l$
[p] $P6/m$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b},\mathbf{c}$ $p=q^2-qr+r^2=$ prime $=6n+1$; $q,r=1,2,\ldots;\ q>r;\ u=1,\ldots,p-1$	$\frac{1}{p}((q-r)x+ry)$, $\frac{1}{p}(-rx+qy),z;+(\frac{ur}{p},\frac{uq}{p},0)$	$1a;$ $\frac{p-1}{6}\times6j$	$1b;$ $\frac{p-1}{6}\times6k$	$2c;$ $\frac{p-1}{3}\times6j$ $4h;$ $\frac{p-1}{3}\times12l$	$2d;$ $\frac{p-1}{3}\times6k$ $6i;$ $\frac{p-1}{2}\times12l$	$2e;$ $\frac{p-1}{6}\times12l$ $p\times6j$	$3f;$ $\frac{p-1}{2}\times6j$ $p\times6k$	$3g;$ $\frac{p-1}{2}\times6k$ $p\times12l$
[4] $P6/m$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z;+(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);+(\frac{1}{2},\frac{1}{2},0)$	$1a;3f$	$1b;3g$	$2c;6j$ $4h;12l$	$2d;6k$ $2\times12l$	$2e;6i$ $4\times6j$	$2\times6j$ $4\times6k$	$2\times6k$ $4\times12l$
[p^2] $P6/m$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=$ prime $=6n-1$; $u,v=1,\ldots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z;\ +(\frac{u}{p},\frac{v}{p},0)$	$1a;$ $\frac{p^2-1}{6}\times6j$	$1b;$ $\frac{p^2-1}{6}\times6k$	$2c;$ $\frac{p^2-1}{3}\times6j$ $4h;$ $\frac{p^2-1}{3}\times12l$	$2d;$ $\frac{p^2-1}{3}\times6k$ $6i;$ $\frac{p^2-1}{2}\times12l$	$2e;$ $\frac{p^2-1}{6}\times12l$ $p^2\times6j$	$3f;$ $\frac{p^2-1}{2}\times6j$ $p^2\times6k$	$3g;$ $\frac{p^2-1}{2}\times6k$ $p^2\times12l$

$P6_3/m$ No. 176 C_{6h}^2

	Axes	Coordinates	Wyckoff positions $2a$	 $2b$	 $2c$	 $2d$ $6g$	 $4e$ $6h$	 $4f$ $12i$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{6}$ (174)		$x,y,z+\frac{1}{4}$	$1a$; $1b$	$2g$	$1d$; $1e$	$1c$; $1f$ $6l$	$2\times 2g$ $3j$; $3k$	$2h$; $2i$ $2\times 6l$
[2] $P6_3$ (173)			$2a$	$2a$	$2b$	$2b$ $6c$	$2\times 2a$ $6c$	$2\times 2b$ $2\times 6c$
[2] $P\bar{3}$ (147)			$2c$	$1a$; $1b$	$2d$	$2d$ $3e$; $3f$	$2\times 2c$ $6g$	$2\times 2d$ $2\times 6g$
[3] $P112_1/m$ (11)			$2e$	$2a$	$2e$	$2e$ $2b$; $2c$; $2d$	$4f$ $3\times 2e$	$4f$ $3\times 4f$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**								
[3] $P6_3/m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$	$2b$; $4e$	$2d$; $4f$	$2c$; $4f$ $6g$; $12i$	$3\times 4e$ $6h$; $12i$	$3\times 4f$ $3\times 12i$
[p] $P6_3/m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime > 2; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times 4e$	$2b$; $\frac{p-1}{2}\times 4e$	$2c(d^*)$; $\frac{p-1}{2}\times 4f$	$2d(c^*)$; $\frac{p-1}{2}\times 4f$ $6g$; $\frac{p-1}{2}\times 12i$	$p\times 4e$ $6h$; $\frac{p-1}{2}\times 12i$	$p\times 4f$ $p\times 12i$
[3] $P6_3/m$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a$; $2c$; $2d$	$2b$; $4f$	$6h$	$6h$ $6g$; $12i$	$4e$; $2\times 4f$ $3\times 6h$	$12i$ $3\times 12i$
[7] $P6_3/m$	$3\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(2x+y), \frac{1}{7}(-x+3y), z$; $\pm(\frac{1}{7},\frac{3}{7},0)$; $\pm(\frac{3}{7},\frac{2}{7},0)$; $\pm(\frac{5}{7},\frac{1}{7},0)$	$2a$; $2\times 6h$	$2b$; $12i$	$2c$; $2\times 6h$	$2d$; $2\times 6h$ $6g$; $3\times 12i$	$4e$; $2\times 12i$ $7\times 6h$	$4f$; $2\times 12i$ $7\times 12i$
[7] $P6_3/m$	$3\mathbf{a}+2\mathbf{b}$, $-2\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{7}(x+2y), \frac{1}{7}(-2x+3y), z$; $\pm(\frac{2}{7},\frac{3}{7},0)$; $\pm(\frac{3}{7},\frac{1}{7},0)$; $\pm(\frac{1}{7},\frac{5}{7},0)$	$2a$; $2\times 6h$	$2b$; $12i$	$2d$; $2\times 6h$	$2c$; $2\times 6h$ $6g$; $3\times 12i$	$4e$; $2\times 12i$ $7\times 6h$	$4f$; $2\times 12i$ $7\times 12i$
[p] $P6_3/m$	$q\mathbf{a}+r\mathbf{b}$, $-r\mathbf{a}+(q-r)\mathbf{b}, \mathbf{c}$ p = prime = $q^2-qr+r^2 = 6n+1$; $q,r = 1,2,\ldots$; $q > r$; $u = 1,\ldots,p-1$	$\frac{1}{p}((q-r)x+ry)$, $\frac{1}{p}(-rx+qy), z$; $+(\frac{ur}{p},\frac{uq}{p},0)$	$2a$; $\frac{p-1}{3}\times 6h$	$2b$; $\frac{p-1}{6}\times 12i$	$2c(d^\dagger)$; $\frac{p-1}{3}\times 6h$	$2d(c^\dagger)$; $\frac{p-1}{3}\times 6h$ $6g$; $\frac{p-1}{2}\times 12i$	$4e$; $\frac{p-1}{3}\times 12i$ $p\times 6h$	$4f$; $\frac{p-1}{3}\times 12i$ $p\times 12i$
[4] $P6_3/m$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6h$	$2b$; $6g$	$2d$; $6h$	$2c$; $6h$ $2\times 12i$	$4e$; $12i$ $4\times 6h$	$4f$; $12i$ $4\times 12i$
[p^2] $P6_3/m$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime $= 6n-1$; $u,v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a$; $\frac{p^2-1}{3}\times 6h$	$2b$; $\frac{p^2-1}{6}\times 12i$	$2d$; $\frac{p^2-1}{3}\times 6h$	$2c$; $\frac{p^2-1}{3}\times 6h$ $6g$; $\frac{p^2-1}{2}\times 12i$	$4e$; $\frac{p^2-1}{3}\times 12i$ $p^2\times 6h$	$4f$; $\frac{p^2-1}{3}\times 12i$ $p^2\times 12i$

* $p = 4n-1$ † $q+r = 3n-1$

D_6^1 No. 177 $P622$

Subgroup	Axes	Coordinates	Wyckoff positions $1a$ $4h$	$1b$ $6i$	$2c$ $6j$	$2d$ $6k$	$2e$ $6l$	$3f$ $6m$	$3g$ $12n$
I Maximal *translationengleiche* subgroups									
[2] $P6$ (168)			$1a$ $2\times2b$	$1a$ $2\times3c$	$2b$ $6d$	$2b$ $6d$	$2\times1a$ $6d$	$3c$ $6d$	$3c$ $2\times6d$
[2] $P321$ (150)			$1a$ $2\times2d$	$1b$ $6g$	$2d$ $2\times3e$	$2d$ $2\times3f$	$2c$ $6g$	$3e$ $6g$	$3f$ $2\times6g$
[2] $P312$ (149)			$1a$ $2h;2i$	$1b$ $6l$	$1c;1e$ $6l$	$1d;1f$ $6l$	$2g$ $2\times3j$	$3j$ $2\times3k$	$3k$ $2\times6l$
[3] $C222$ (21)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$2a$ $8l$	$2d$ $4j;2\times4k$	$4g$ $4e;8l$	$4h$ $4f;8l$	$4i$ $4g;8l$	$2b;4k$ $4h;8l$	$2c;4k$ $3\times8l$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$							
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$							
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $P6_322$ (182)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$2a$ $2\times4f$	$2b$ $12i$	$4f$ $2\times6g$	$2c;2d$ $12i$	$4e$ $12i$	$6g$ $2\times6h$	$6h$ $2\times12i$
[2] $P6_322$ (182)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2b$ $2\times4f$	$2a$ $12i$	$2c;2d$ $12i$	$4f$ $2\times6g$	$4e$ $2\times6h$	$6h$ $12i$	$6g$ $2\times12i$
[3] $P6_422$ (181)	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3a$ $12k$	$3b$ $3\times6f$	$6i$ $6g;12k$	$6j$ $6h;12k$	$6e$ $6i;12k$	$3c;6f$ $6j;12k$	$3d;6f$ $3\times12k$
[3] $P6_222$ (180)	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$3a$ $12k$	$3b$ $3\times6f$	$6i$ $6g;12k$	$6j$ $6h;12k$	$6e$ $6i;12k$	$3c;6f$ $6j;12k$	$3d;6f$ $3\times12k$
Enlarged unit cell, isomorphic									
[2] $P622$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a;1b$ $2\times4h$	$2e$ $2\times6i$	$2c;2d$ $6j;6k$	$4h$ $12n$	$2\times2e$ $6l;6m$	$3f;3g$ $12n$	$6i$ $2\times12n$
[2] $P622$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2e$ $2\times4h$	$1a;1b$ $2\times6i$	$4h$ $12n$	$2c;2d$ $6j;6k$	$2\times2e$ $12n$	$6i$ $6l;6m$	$3f;3g$ $2\times12n$
[3] $P622$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a;2e$ $3\times4h$	$1b;2e$ $3\times6i$	$2c;4h$ $6j;12n$	$2d;4h$ $6k;12n$	$3\times2e$ $6l;12n$	$3f;6i$ $6m;12n$	$3g;6i$ $3\times12n$
[p] $P622$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$ p = prime > 2; $u = 1,\ldots,p-1$	$1a;\frac{p-1}{2}\times2e$ $p\times4h$	$1b;\frac{p-1}{2}\times2e$ $p\times6i$	$2c;\frac{p-1}{2}\times4h$ $6j;\frac{p-1}{2}\times12n$	$2d;\frac{p-1}{2}\times4h$ $6k;\frac{p-1}{2}\times12n$	$p\times2e$ $6l;\frac{p-1}{2}\times12n$	$3f;\frac{p-1}{2}\times6i$ $6m;\frac{p-1}{2}\times12n$	$3g;\frac{p-1}{2}\times6i$ $p\times12n$
[3] $P622$	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y)$, $\frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;2c$ $12n$	$1b;2d$ $6i;12n$	$6j$ $3\times6l$	$6k$ $3\times6m$	$2e;4h$ $6j;12n$	$3f;6l$ $6k;12n$	$3g;6m$ $3\times12n$
[4] $P622$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$1a;3f$ $4h;12n$	$1b;3g$ $2\times12n$	$2c;6l$ $2\times6j;12n$	$2d;6m$ $2\times6k;12n$	$2e;6i$ $2\times6l;12n$	$6j;6l$ $2\times6m;12n$	$6k;6m$ $4\times12n$
[p^2] $P622$	p**a**, p**b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$ p = prime > 4; $u,v = 1,\ldots,p-1$	$1a;\frac{p-1}{2}\times6j$; $\frac{p-1}{2}\times6l$; $\frac{(p-1)(p-5)}{12}\times12n$ $4h$; $\frac{p^2-1}{3}\times12n$	$1b;\frac{p-1}{2}\times6k$; $\frac{p-1}{2}\times6m$; $\frac{(p-1)(p-5)}{12}\times12n$ $6i$; $\frac{p^2-1}{2}\times12n$	$2c$; $(p-1)\times6l$; $\frac{(p-1)(p-2)}{6}\times12n$ $p\times6j$; $\frac{p(p-1)}{2}\times12n$	$2d$; $(p-1)\times6m$; $\frac{(p-1)(p-2)}{6}\times12n$ $p\times6k$; $\frac{p(p-1)}{2}\times12n$	$2e;\frac{p^2-1}{6}\times12n$ $p\times6l$; $\frac{p(p-1)}{2}\times12n$	$3f;\frac{p-1}{2}\times6j$; $\frac{p-1}{2}\times6l$; $\frac{(p-1)^2}{4}\times12n$ $p\times6m$; $\frac{p(p-1)}{2}\times12n$	$3g;\frac{p-1}{2}\times6k$; $\frac{p-1}{2}\times6m$; $\frac{(p-1)^2}{4}\times12n$ $p^2\times12n$

$P6_122$ No. 178 D_6^2

Axes	Coordinates	Wyckoff positions		
		$6a$	$6b$	$12c$
I Maximal *translationengleiche* subgroups				
[2] $P6_1$ (169)		$6a$	$6a$	$2\times6a$
[2] $P3_121$ (152)	$x,y,z-\frac{1}{6}$	$3a$; $3b$	$6c$	$2\times6c$
[2] $P3_112$ (151)	$x,y,z-\frac{1}{12}$	$6c$	$3a$; $3b$	$2\times6c$
[3] $C222_1$ (20) **a**, **a**+2**b**, **c**	$x-\frac{1}{2}y,\frac{1}{2}y,z$	$4a$; $8c$	$4b$; $8c$	$3\times8c$
conjugate: **b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y,-\frac{1}{2}x,z+\frac{1}{6}$			
conjugate: −**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y),\frac{1}{2}(x-y),z-\frac{1}{6}$			
alternative:				
$C222_1$ 2**a**+**b**, **b**, **c**	$\frac{1}{2}x,-\frac{1}{2}x+y,z-\frac{1}{12}$	$4b$; $8c$	$4a$; $8c$	$3\times8c$
or **a**+2**b**, −**a**, **c**	$\frac{1}{2}y,-x+\frac{1}{2}y,z-\frac{1}{4}$			
or **a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y),\frac{1}{2}(x+y),z+\frac{1}{12}$			
II Maximal *klassengleiche* subgroups				
Enlarged unit cell, isomorphic				
[5] $P6_522$ (179) **a**, **b**, 5**c**	$x,y,\frac{1}{5}z$; $\pm(0,0,\frac{1}{5})$; $\pm(0,0,\frac{2}{5})$	$6a$; $2\times12c$	$6b$; $2\times12c$	$5\times12c$
[p] $P6_522$ (179) **a**, **b**, p**c** p = prime = $6n-1$; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$6a$; $\frac{p-1}{2}\times12c$	$6b$; $\frac{p-1}{2}\times12c$	$p\times12c$
[7] $P6_122$ **a**, **b**, 7**c**	$x,y,\frac{1}{7}z$; $\pm(0,0,\frac{1}{7})$; $\pm(0,0,\frac{2}{7})$; $\pm(0,0,\frac{3}{7})$	$6a$; $3\times12c$	$6b$; $3\times12c$	$7\times12c$
[p] $P6_122$ **a**, **b**, p**c** p = prime = $6n+1$; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$6a$; $\frac{p-1}{2}\times12c$	$6b$; $\frac{p-1}{2}\times12c$	$p\times12c$
[3] $P6_122$ 2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y),z-\frac{1}{12}$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$3\times6b$	$6a$; $12c$	$3\times12c$
[4] $P6_122$ 2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2\times6a$; $12c$	$2\times6b$; $12c$	$4\times12c$
[p^2] $P6_122$ p**a**, p**b**, **c** p = prime $\neq 3$; $u,v=1,\ldots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$p\times6a$; $\frac{p(p-1)}{2}\times12c$	$p\times6b$; $\frac{p(p-1)}{2}\times12c$	$p^2\times12c$

D_6^3 No. 179 $P6_522$

	Axes	Coordinates	Wyckoff positions 6*a*	6*b*	12*c*
I Maximal *translationengleiche* subgroups					
[2] $P6_5$ (170)			6*a*	6*a*	$2\times 6a$
[2] $P3_221$ (154)		$x, y, z+\frac{1}{6}$	3*a*; 3*b*	6*c*	$2\times 6c$
[2] $P3_212$ (153)		$x, y, z+\frac{1}{12}$	6*c*	3*a*; 3*b*	$2\times 6c$
[3] $C222_1$ (20)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	4*a*; 8*c*	4*b*; 8*c*	$3\times 8c$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z-\frac{1}{6}$			
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z+\frac{1}{6}$			
alternative:					
$C222_1$	2**a**+**b**, **b**, **c**	$\frac{1}{2}x, -\frac{1}{2}x+y, z+\frac{1}{12}$	4*b*; 8*c*	4*a*; 8*c*	$3\times 8c$
	or **a**+2**b**, −**a**, **c**	$\frac{1}{2}y, -x+\frac{1}{2}y, z+\frac{1}{4}$			
	or **a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z-\frac{1}{12}$			
II Maximal *klassengleiche* subgroups					
Enlarged unit cell, isomorphic					
[5] $P6_122$ (178)	**a**, **b**, 5**c**	$x, y, \frac{1}{5}z$; $\pm(0,0,\frac{1}{5})$; $\pm(0,0,\frac{2}{5})$	6*a*; $2\times 12c$	6*b*; $2\times 12c$	$5\times 12c$
[*p*] $P6_122$ (178)	**a**, **b**, *p***c**	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	6*a*; $\frac{p-1}{2}\times 12c$	6*b*; $\frac{p-1}{2}\times 12c$	$p\times 12c$
	$p=\text{prime}=6n-1$; $u=1,\dots,p-1$				
[7] $P6_522$	**a**, **b**, 7**c**	$x, y, \frac{1}{7}z$; $\pm(0,0,\frac{1}{7})$; $\pm(0,0,\frac{2}{7})$; $\pm(0,0,\frac{3}{7})$	6*a*; $3\times 12c$	6*b*; $3\times 12c$	$7\times 12c$
[*p*] $P6_522$	**a**, **b**, *p***c**	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	6*a*; $\frac{p-1}{2}\times 12c$	6*b*; $\frac{p-1}{2}\times 12c$	$p\times 12c$
	$p=\text{prime}=6n+1$; $u=1,\dots,p-1$				
[3] $P6_522$	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z+\frac{1}{12}$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$3\times 6b$	6*a*; 12*c*	$3\times 12c$
[4] $P6_522$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2\times 6a$; 12*c*	$2\times 6b$; 12*c*	$4\times 12c$
[p^2] $P6_522$	*p***a**, *p***b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$p\times 6a$; $\frac{p(p-1)}{2}\times 12c$	$p\times 6b$; $\frac{p(p-1)}{2}\times 12c$	$p^2\times 12c$
	$p=\text{prime}\neq 3$; $u,v=1,\dots,p-1$				

$P6_222$ No. 180 D_6^4

Subgroup	Axes	Coordinates	Wyckoff positions: $3a$	$3b$ $6g$	$3c$ $6h$	$3d$ $6i$	$6e$ $6j$	$6f$ $12k$
I Maximal *translationengleiche* subgroups								
[2] $P6_2$ (171)			$3a$	$3a$ $6c$	$3b$ $6c$	$3b$ $6c$	$2{\times}3a$ $6c$	$2{\times}3b$ $2{\times}6c$
[2] $P3_221$ (154)		$x,y,z-\frac{1}{3}$	$3a$	$3b$ $2{\times}3a$	$3a$ $2{\times}3b$	$3b$ $6c$	$6c$ $6c$	$6c$ $2{\times}6c$
[2] $P3_212$ (153)		$x,y,z+\frac{1}{3}$	$3a$	$3b$ $6c$	$3a$ $6c$	$3b$ $2{\times}3a$	$6c$ $2{\times}3b$	$6c$ $2{\times}6c$
[3] $C222$ (21)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$2a;4i$	$2d;4i$ $4e;8l$	$2b;4k$ $4f;8l$	$2c;4k$ $4g;8l$	$3{\times}4i$ $4h;8l$	$4j;2{\times}4k$ $3{\times}8l$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z+\frac{1}{3}$						
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z-\frac{1}{3}$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P6_122$ (178)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$6a$	$6b$ $2{\times}6a$	$6a$ $12c$	$6b$ $12c$	$12c$ $2{\times}6b$	$12c$ $2{\times}12c$
[2] $P6_122$ (178)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$6b$	$6a$ $12c$	$6b$ $2{\times}6a$	$6a$ $2{\times}6b$	$12c$ $12c$	$12c$ $2{\times}12c$
Enlarged unit cell, isomorphic								
[2] $P6_422$ (181)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$3a;3b$	$6e$ $6g;6h$	$3c;3d$ $12k$	$6f$ $6i;6j$	$2{\times}6e$ $12k$	$2{\times}6f$ $2{\times}12k$
[2] $P6_422$ (181)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$6e$	$3a;3b$ $12k$	$6f$ $6g;6h$	$3c;3d$ $12k$	$2{\times}6e$ $6i;6j$	$2{\times}6f$ $2{\times}12k$
[5] $P6_422$ (181)	$\mathbf{a}, \mathbf{b}, 5\mathbf{c}$	$x,y,\frac{1}{5}z;\ \pm(0,0,\frac{1}{5});$ $\pm(0,0,\frac{2}{5})$	$3a;2{\times}6e$	$3b;2{\times}6e$ $6g;2{\times}12k$	$3c;2{\times}6f$ $6h;2{\times}12k$	$3d;2{\times}6f$ $6i;2{\times}12k$	$5{\times}6e$ $6j;2{\times}12k$	$5{\times}6f$ $5{\times}12k$
[p] $P6_422$ (181)	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p=\text{prime}=6n-1;\ u=1,\ldots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$3a;\frac{p-1}{2}{\times}6e$	$3b;\frac{p-1}{2}{\times}6e$ $6g;\frac{p-1}{2}{\times}12k$	$3c;\frac{p-1}{2}{\times}6f$ $6h;\frac{p-1}{2}{\times}12k$	$3d;\frac{p-1}{2}{\times}6f$ $6i;\frac{p-1}{2}{\times}12k$	$p{\times}6e$ $6j;\frac{p-1}{2}{\times}12k$	$p{\times}6f$ $p{\times}12k$
[7] $P6_222$	$\mathbf{a}, \mathbf{b}, 7\mathbf{c}$	$x,y,\frac{1}{7}z;\ \pm(0,0,\frac{1}{7})$ $\pm(0,0,\frac{2}{7});\pm(0,0,\frac{3}{7})$	$3a;3{\times}6e$	$3b;3{\times}6e$ $6g;3{\times}12k$	$3c;3{\times}6f$ $6h;3{\times}12k$	$3d;3{\times}6f$ $6i;3{\times}12k$	$7{\times}6e$ $6j;3{\times}12k$	$7{\times}6f$ $7{\times}12k$
[p] $P6_222$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ $p=\text{prime}=6n+1;\ u=1,\ldots,p-1$	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$3a;\frac{p-1}{2}{\times}6e$	$3b;\frac{p-1}{2}{\times}6e$ $6g;\frac{p-1}{2}{\times}12k$	$3c;\frac{p-1}{2}{\times}6f$ $6h;\frac{p-1}{2}{\times}12k$	$3d;\frac{p-1}{2}{\times}6f$ $6i;\frac{p-1}{2}{\times}12k$	$p{\times}6e$ $6j;\frac{p-1}{2}{\times}12k$	$p{\times}6f$ $p{\times}12k$
[3] $P6_222$	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y),$ $z+\frac{1}{3};\pm(\frac{1}{3},\frac{2}{3},0)$	$3a;6i$	$3b;6j$ $3{\times}6i$	$3c;6i$ $3{\times}6j$	$3d;6j$ $6g;12k$	$6e;12k$ $6h;12k$	$6f;12k$ $3{\times}12k$
[4] $P6_222$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z;+(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);+(\frac{1}{2},\frac{1}{2},0)$	$3a;3c;6f$	$3b;3d;6f$ $2{\times}6g;12k$	$6g;6i$ $2{\times}6h;12k$	$6h;6j$ $2{\times}6i;12k$	$6e;3{\times}6f$ $2{\times}6j;12k$	$2{\times}12k$ $4{\times}12k$
[p^2] $P6_222$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ $p=\text{prime}>4;$	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$3a;\frac{p-1}{2}{\times}6g;$ $\frac{p-1}{2}{\times}6i;$ $\frac{(p-1)^2}{4}{\times}12k$	$3b;\frac{p-1}{2}{\times}6h;$ $\frac{p-1}{2}{\times}6j;$ $\frac{(p-1)^2}{4}{\times}12k$ $p{\times}6g;$ $\frac{p(p-1)}{2}{\times}12k$	$3c;\frac{p-1}{2}{\times}6g;$ $\frac{p-1}{2}{\times}6i;$ $\frac{(p-1)^2}{4}{\times}12k$ $p{\times}6h;$ $\frac{p(p-1)}{2}{\times}12k$	$3d;\frac{p-1}{2}{\times}6h;$ $\frac{p-1}{2}{\times}6j;$ $\frac{(p-1)^2}{4}{\times}12k$ $p{\times}6i;$ $\frac{p(p-1)}{2}{\times}12k$	$6e;\frac{p^2-1}{2}{\times}12k$ $p{\times}6j;$ $\frac{p(p-1)}{2}{\times}12k$	$6f;\frac{p^2-1}{2}{\times}12k$ $p^2{\times}12k$

D_6^5 No. 181 $P6_422$

Subgroup	Axes	Coordinates	Wyckoff positions					
			$3a$	$3b$ $6g$	$3c$ $6h$	$3d$ $6i$	$6e$ $6j$	$6f$ $12k$
I Maximal *translationengleiche* subgroups								
[2] $P6_4$ (172)			$3a$	$3a$ $6c$	$3b$ $6c$	$3b$ $6c$	$2\times3a$ $6c$	$2\times3b$ $2\times6c$
[2] $P3_121$ (152)		$x,y,z+\frac{1}{3}$	$3a$	$3b$ $2\times3a$	$3a$ $2\times3b$	$3b$ $6c$	$6c$ $6c$	$6c$ $2\times6c$
[2] $P3_112$ (151)		$x,y,z-\frac{1}{3}$	$3a$	$3b$ $6c$	$3a$ $6c$	$3b$ $2\times3a$	$6c$ $2\times3b$	$6c$ $2\times6c$
[3] $C222$ (21)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y,\frac{1}{2}y,z$	$2a;4i$	$2d;4i$ $4e;8l$	$2b;4k$ $4f;8l$	$2c;4k$ $4g;8l$	$3\times4i$ $4h;8l$	$4j;2\times4k$ $3\times8l$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y,-\frac{1}{2}x,z-\frac{1}{3}$						
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y),\frac{1}{2}(x-y),z+\frac{1}{3}$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P6_522$ (179)	**a**,**b**,2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$6a$	$6b$ $2\times6a$	$6a$ $12c$	$6b$ $12c$	$12c$ $2\times6b$	$12c$ $2\times12c$
[2] $P6_522$ (179)	**a**,**b**,2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$6b$	$6a$ $12c$	$6b$ $2\times6a$	$6a$ $2\times6b$	$12c$ $12c$	$12c$ $2\times12c$
Enlarged unit cell, isomorphic								
[2] $P6_222$ (180)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$3a;3b$	$6e$ $6g;6h$	$3c;3d$ $12k$	$6f$ $6i;6j$	$2\times6e$ $12k$	$2\times6f$ $2\times12k$
[2] $P6_222$ (180)	**a**, **b**, 2**c**	$x,y,\frac{1}{2}z+\frac{1}{4};+(0,0,\frac{1}{2})$	$6e$	$3a;3b$ $12k$	$6f$ $6g;6h$	$3c;3d$ $12k$	$2\times6e$ $6i;6j$	$2\times6f$ $2\times12k$
[5] $P6_222$ (180)	**a**, **b**, 5**c**	$x,y,\frac{1}{5}z;\pm(0,0,\frac{1}{5})$; $\pm(0,0,\frac{2}{5})$	$3a;2\times6e$	$3b;2\times6e$ $6g;2\times12k$	$3c;2\times6f$ $6h;2\times12k$	$3d;2\times6f$ $6i;2\times12k$	$5\times6e$ $6j;2\times12k$	$5\times6f$ $5\times12k$
[p] $P6_222$ (180)	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;\ +(0,0,\frac{u}{p})$ $p=\text{prime}=6n-1;\ u=1,\dots,p-1$	$3a;\frac{p-1}{2}\times6e$	$3b;\frac{p-1}{2}\times6e$ $6g;\frac{p-1}{2}\times12k$	$3c;\frac{p-1}{2}\times6f$ $6h;\frac{p-1}{2}\times12k$	$3d;\frac{p-1}{2}\times6f$ $6i;\frac{p-1}{2}\times12k$	$p\times6e$ $6j;\frac{p-1}{2}\times12k$	$p\times6f$ $p\times12k$
[7] $P6_422$	**a**, **b**, 7**c**	$x,y,\frac{1}{7}z;\ \pm(0,0,\frac{1}{7})$ $\pm(0,0,\frac{2}{7});\pm(0,0,\frac{3}{7})$	$3a;3\times6e$	$3b;3\times6e$ $6g;3\times12k$	$3c;3\times6f$ $6h;3\times12k$	$3d;3\times6f$ $6i;3\times12k$	$7\times6e$ $6j;3\times12k$	$7\times6f$ $7\times12k$
[p] $P6_422$	**a**, **b**, p**c**	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$ $p=\text{prime}=6n+1;\ u=1,\dots,p-1$	$3a;\frac{p-1}{2}\times6e$	$3b;\frac{p-1}{2}\times6e$ $6g;\frac{p-1}{2}\times12k$	$3c;\frac{p-1}{2}\times6f$ $6h;\frac{p-1}{2}\times12k$	$3d;\frac{p-1}{2}\times6f$ $6i;\frac{p-1}{2}\times12k$	$p\times6e$ $6j;\frac{p-1}{2}\times12k$	$p\times6f$ $p\times12k$
[3] $P6_422$	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y)$, $z-\frac{1}{3};\pm(\frac{1}{3},\frac{2}{3},0)$	$3a;6i$	$3b;6j$ $3\times6i$	$3c;6i$ $3\times6j$	$3d;6j$ $6g;12k$	$6e;12k$ $6h;12k$	$6f;12k$ $3\times12k$
[4] $P6_422$	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z;+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0);+(\frac{1}{2},\frac{1}{2},0)$	$3a;3c;6f$	$3b;3d;6f$ $2\times6g;12k$	$6g;6i$ $2\times6h;12k$	$6h;6j$ $2\times6i;12k$	$6e;3\times6f$ $2\times6j;12k$	$2\times12k$ $4\times12k$
[p^2] $P6_422$	p**a**, p**b**, **c**	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>4$; $u,v=1,\dots,p-1$	$3a;\frac{p-1}{2}\times6g$; $\frac{p-1}{2}\times6i$; $\frac{(p-1)^2}{4}\times12k$	$3b;\frac{p-1}{2}\times6h$; $\frac{p-1}{2}\times6j$; $\frac{(p-1)^2}{4}\times12k$ $p\times6g$; $\frac{p(p-1)}{2}\times12k$	$3c;\frac{p-1}{2}\times6g$; $\frac{p-1}{2}\times6i$; $\frac{(p-1)^2}{4}\times12k$ $p\times6h$; $\frac{p(p-1)}{2}\times12k$	$3d;\frac{p-1}{2}\times6h$; $\frac{p-1}{2}\times6j$; $\frac{(p-1)^2}{4}\times12k$ $p\times6i$; $\frac{p(p-1)}{2}\times12k$	$6e;\frac{p^2-1}{2}\times12k$ $p\times6j$; $\frac{p(p-1)}{2}\times12k$	$6f;\frac{p^2-1}{2}\times12k$ $p^2\times12k$

$P6_322$ No. 182 D_6^6

	Axes	Coordinates	Wyckoff positions					
			$2a$	$2b$	$2c$	$2d$ $6g$	$4e$ $6h$	$4f$ $12i$
I Maximal *translationengleiche* subgroups								
[2] $P6_3$ (173)			$2a$	$2a$	$2b$	$2b$ $6c$	$2\times2a$ $6c$	$2\times2b$ $2\times6c$
[2] $P321$ (150)			$1a$; $1b$	$2c$	$2d$	$2d$ $3e$; $3f$	$2\times2c$ $6g$	$2\times2d$ $2\times6g$
[2] $P312$ (149)		$x,y,z+\frac{1}{4}$	$2g$	$1a$; $1b$	$1d$; $1e$	$1c$; $1f$ $6l$	$2\times2g$ $3j$; $3k$	$2h$; $2i$ $2\times6l$
[3] $C222_1$ (20)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$4a$	$4b$	$4b$	$4b$ $4a$; $8c$	$8c$ $4b$; $8c$	$8c$ $3\times8c$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$						
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$						
alternative: $C222_1$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z+\frac{1}{4}$	$4b$	$4a$	$4a$	$4a$ $4b$; $8c$	$8c$ $4a$; $8c$	$8c$ $3\times8c$
or	$\mathbf{a}+2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z+\frac{1}{4}$						
or	$\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z+\frac{1}{4}$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[3] $P6_522$ (179)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$6a$	$6b$	$6b$	$6b$ $6a$; $12c$	$12c$ $6b$; $12c$	$12c$ $3\times12c$
[3] $P6_122$ (178)	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$6a$	$6b$	$6b$	$6b$ $6a$; $12c$	$12c$ $6b$; $12c$	$12c$ $3\times12c$
Enlarged unit cell, isomorphic								
[3] $P6_322$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$	$2b$; $4e$	$2d$; $4f$	$2c$; $4f$ $6g$; $12i$	$3\times4e$ $6h$; $12i$	$3\times4f$ $3\times12i$
[p] $P6_322$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$ p = prime > 2; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times4e$	$2b$; $\frac{p-1}{2}\times4e$	$2c(d^*)$; $\frac{p-1}{2}\times4f$	$2d(c^*)$; $\frac{p-1}{2}\times4f$ $6g$; $\frac{p-1}{2}\times12i$	$p\times4e$ $6h$; $\frac{p-1}{2}\times12i$	$p\times4f$ $p\times12i$
[3] $P6_322$	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z+\frac{1}{4}$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2b$; $2c$; $2d$	$2a$; $4f$	$6g$	$6g$ $3\times6h$	$4e$; $2\times4f$ $6g$; $12i$	$12i$ $3\times12i$
[4] $P6_322$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6g$	$2b$; $6h$	$2d$; $6h$	$2c$; $6h$ $2\times6g$; $12i$	$4e$; $12i$ $2\times6h$; $12i$	$4f$; $12i$ $4\times12i$
[p^2] $P6_322$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ p = prime $\neq 3$; $u,v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a$; $(p-1)\times6g$; $\frac{(p-1)(p-2)}{6}\times12i$	$2b$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12i$	$2c(d^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12i$	$2d(c^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12i$ $p\times6g$; $\frac{p(p-1)}{2}\times12i$	$4e$; $\frac{p^2-1}{3}\times12i$ $p\times6h$; $\frac{p(p-1)}{2}\times12i$	$4f$; $\frac{p^2-1}{3}\times12i$ $p^2\times12i$

$^*\ p = 4n-1$ $\quad$ $^\dagger\ p = 3n-1$

C_{6v}^{1} No. 183 $P6mm$

	Axes	Coordinates	$1a$	$2b$	$3c$	$6d$	$6e$	$12f$
I Maximal *translationengleiche* subgroups								
[2] $P6$ (168)			$1a$	$2b$	$3c$	$6d$	$6d$	$2\times 6d$
[2] $P31m$ (157)			$1a$	$2b$	$3c$	$2\times 3c$	$6d$	$2\times 6d$
[2] $P3m1$ (156)			$1a$	$1b; 1c$	$3d$	$6e$	$2\times 3d$	$2\times 6e$
[3] $Cmm2$ (35)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$2a$	$4e$	$2b; 4c$	$4d; 8f$	$4e; 8f$	$3\times 8f$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$						
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$						
alternative:								
$Cmm2$	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	$2a$	$4d$	$2b; 4c$	$4e; 8f$	$4d; 8f$	$3\times 8f$
	or $\mathbf{a}+2\mathbf{b}, -\mathbf{a}, \mathbf{c}$	$\frac{1}{2}y, -x+\frac{1}{2}y, z$						
	or $\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P6_3mc$ (186)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a$	$2\times 2b$	$6c$	$12d$	$2\times 6c$	$2\times 12d$
[2] $P6_3cm$ (185)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a$	$4b$	$6c$	$2\times 6c$	$12d$	$2\times 12d$
[2] $P6cc$ (184)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2a$	$4b$	$6c$	$12d$	$12d$	$2\times 12d$
Enlarged unit cell, isomorphic								
[2] $P6mm$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z;\ +(0,0,\frac{1}{2})$	$2\times 1a$	$2\times 2b$	$2\times 3c$	$2\times 6d$	$2\times 6e$	$2\times 12f$
[3] $P6mm$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z;\ \pm(0,0,\frac{1}{3})$	$3\times 1a$	$3\times 2b$	$3\times 3c$	$3\times 6d$	$3\times 6e$	$3\times 12f$
[p] $P6mm$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z;\ +(0,0,\frac{u}{p})$	$p\times 1a$	$p\times 2b$	$p\times 3c$	$p\times 6d$	$p\times 6e$	$p\times 12f$
	p = prime; $u = 1,\ldots,p-1$							
[3] $P6mm$	$2\mathbf{a}+\mathbf{b}, -\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z+\frac{1}{3};\ \pm(\frac{1}{3},\frac{2}{3},0)$	$1a; 2b$	$6d$	$3c; 6e$	$3\times 6e$	$6d; 12f$	$3\times 12f$
[4] $P6mm$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z;\ +(\frac{1}{2},0,0);\ +(0,\frac{1}{2},0);\ +(\frac{1}{2},\frac{1}{2},0)$	$1a; 3c$	$2b; 6e$	$6d; 6e$	$2\times 6d; 12f$	$2\times 6e; 12f$	$4\times 12f$
[p^2] $P6mm$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$; p = prime > 4;	$\frac{1}{p}x, \frac{1}{p}y, z;\ +(\frac{u}{p},\frac{v}{p},0)$; $u, v = 1,\ldots,p-1$	$1a$; $\frac{p-1}{2}\times 6d$; $\frac{p-1}{2}\times 6e$; $\frac{(p-1)(p-5)}{12}\times 12f$	$2b$; $(p-1)\times 6e$; $\frac{(p-1)(p-2)}{6}\times 12f$	$3c$; $\frac{p-1}{2}\times 6d$; $\frac{p-1}{2}\times 6e$; $\frac{(p-1)^2}{4}\times 12f$	$p\times 6d$; $\frac{p(p-1)}{2}\times 12f$	$p\times 6e$; $\frac{p(p-1)}{2}\times 12f$	$p^2\times 12f$

*P*6*cc* No. 184 C_{6v}^2

	Axes	Coordinates	Wyckoff positions 2*a*	4*b*	6*c*	12*d*
I Maximal *translationengleiche* subgroups						
[2] *P*6 (168)			2×1*a*	2×2*b*	2×3*c*	2×6*d*
[2] *P*31*c* (159)			2*a*	2×2*b*	6*c*	2×6*c*
[2] *P*3*c*1 (158)			2*a*	2*b*; 2*c*	6*d*	2×6*d*
[3] *Ccc*2 (37)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	4*a*	8*d*	4*b*; 2×4*c*	3×8*d*
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$				
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$				
alternative:						
*Ccc*2	2**a**+**b**, **b**, **c**	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	4*a*	8*d*	4*b*; 2×4*c*	3×8*d*
or	**a**+2**b**, −**a**, **c**	$\frac{1}{2}y, -x+\frac{1}{2}y, z$				
or	**a**−**b**, **a**+**b**, **c**	$\frac{1}{2}(x-y), \frac{1}{2}(x+y), z$				
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[3] *P*6*cc*	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	3×2*a*	3×4*b*	3×6*c*	3×12*d*
[*p*] *P*6*cc*	**a**, **b**, *p***c** $p =$ prime > 2; $u = 1,\ldots,p-1$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$	*p*×2*a*	*p*×4*b*	*p*×6*c*	*p*×12*d*
[3] *P*6*cc*	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z; \pm(\frac{1}{3},\frac{2}{3},0)$	2*a*; 4*b*	12*d*	6*c*; 12*d*	3×12*d*
[4] *P*6*cc*	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	2*a*; 6*c*	4*b*; 12*d*	2×12*d*	4×12*d*
$[p^2]$ *P*6*cc*	*p***a**, *p***b**, **c** $p =$ prime > 4; $u, v = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$	$2a; \frac{p^2-1}{6}\times 12d$	$4b; \frac{p^2-1}{3}\times 12d$	$6c; \frac{p^2-1}{2}\times 12d$	$p^2\times 12d$

C_{6v}^{3} No. 185 $P6_3cm$

	Axes	Coordinates	$2a$	$4b$	$6c$	$12d$
I Maximal *translationengleiche* subgroups						
[2] $P6_3$ (173)			$2a$	$2\times2b$	$6c$	$2\times6c$
[2] $P3c1$ (158)			$2a$	$2b$; $2c$	$6d$	$2\times6d$
[2] $P31m$ (157)			$2\times1a$	$2\times2b$	$2\times3c$	$2\times6d$
[3] $Cmc2_1$ (36)	$2\mathbf{a}+\mathbf{b}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	$4a$	$8b$	$4a$; $8b$	$3\times8b$
conjugate:	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{a}-\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(-x+y), -\frac{1}{2}(x+y), z$				
conjugate:	$-\mathbf{a}-2\mathbf{b}$, $\mathbf{a}$, $\mathbf{c}$	$-\frac{1}{2}y, x-\frac{1}{2}y, z$				
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[3] $P6_3mc$ (186)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+2\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), z$; $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	$2a$; $2\times2b$	$12d$	$3\times6c$	$3\times12d$
Enlarged unit cell, isomorphic						
[3] $P6_3cm$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$3\times2a$	$3\times4b$	$3\times6c$	$3\times12d$
[p] $P6_3cm$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$	$p\times2a$	$p\times4b$	$p\times6c$	$p\times12d$
	$p = \text{prime} > 2$; $u = 1, \ldots, p-1$					
[4] $P6_3cm$	$2\mathbf{a}$, $2\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2}, 0, 0)$; $+(0, \frac{1}{2}, 0)$; $+(\frac{1}{2}, \frac{1}{2}, 0)$	$2a$; $6c$	$4b$; $12d$	$2\times6c$; $12d$	$4\times12d$
[p^2] $P6_3cm$	$p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$	$2a$; $(p-1)\times6c$; $\frac{(p-1)(p-2)}{6}\times12d$	$4b$; $\frac{p^2-1}{3}\times12d$	$p\times6c$; $\frac{p(p-1)}{2}\times12d$	$p^2\times12d$
	$p = \text{prime} \neq 3$; $u, v = 1, \ldots, p-1$					

$P6_3mc$ No. 186 C_{6v}^4

	Axes	Coordinates	2a	2b	6c	12d
I Maximal *translationengleiche* subgroups						
[2] $P6_3$ (173)			$2a$	$2b$	$6c$	$2\times6c$
[2] $P31c$ (159)			$2a$	$2b$	$6c$	$2\times6c$
[2] $P3m1$ (156)			$2\times1a$	$1b$; $1c$	$2\times3d$	$2\times6e$
[3] $Cmc2_1$ (36)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$4a$	$4a$	$4a$; $8b$	$3\times8b$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$				
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$				
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, non-isomorphic						
[3] $P6_3cm$ (185)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3}, \frac{2}{3}, 0)$	$2a$; $4b$	$6c$	$6c$; $12d$	$3\times12d$
Enlarged unit cell, isomorphic						
[3] $P6_3mc$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z$; $\pm(0, 0, \frac{1}{3})$	$3\times2a$	$3\times2b$	$3\times6c$	$3\times12d$
[p] $P6_3mc$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$ p = prime > 2; $u = 1, \ldots, p-1$	$p\times2a$	$p\times2b$	$p\times6c$	$p\times12d$
[4] $P6_3mc$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2}, 0, 0)$; $+(0, \frac{1}{2}, 0)$; $+(\frac{1}{2}, \frac{1}{2}, 0)$	$2a$; $6c$	$2b$; $6c$	$2\times6c$; $12d$	$4\times12d$
[p^2] $P6_3mc$	p**a**, p**b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$ p = prime ≠ 3; $u, v = 1, \ldots, p-1$	$2a$; $(p-1)\times6c$; $\frac{(p-1)(p-2)}{6}\times12d$	$2b$; $(p-1)\times6c$; $\frac{(p-1)(p-2)}{6}\times12d$	$p\times6c$; $\frac{p(p-1)}{2}\times12d$	$p^2\times12d$

$P\bar{6}m2$ No. 187

CONTINUED (*from next page*)

	Axes	Coordinates	1a	1b	1c 2h	1d 2i	1e 3j 6m	1f 3k 6n	2g 6l 12o
[p] $P\bar{6}m2$	**a**, **b**, p**c**	$x, y, \frac{1}{p}z$; $+(0, 0, \frac{u}{p})$ p = prime > 2; $u = 1, \ldots, p-1$	$1a$; $\frac{p-1}{2}\times2g$	$1b$; $\frac{p-1}{2}\times2g$	$1c$; $\frac{p-1}{2}\times2h$ $p\times2h$	$1d$; $\frac{p-1}{2}\times2h$ $p\times2i$	$1e$; $\frac{p-1}{2}\times2i$ $3j$; $\frac{p-1}{2}\times6n$ $6m$; $\frac{p-1}{2}\times12o$	$1f$; $\frac{p-1}{2}\times2i$ $3k$; $\frac{p-1}{2}\times6n$ $p\times6n$	$p\times2g$ $6l$; $\frac{p-1}{2}\times12o$ $p\times12o$
[4] $P\bar{6}m2$	2**a**, 2**b**, **c**	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2}, 0, 0)$; $+(0, \frac{1}{2}, 0)$; $+(\frac{1}{2}, \frac{1}{2}, 0)$	$1a$; $3j$	$1b$; $3k$	$1e$; $3j$ $2i$; $6n$	$1f$; $3k$ $2h$; $6n$	$1c$; $3j$ $2\times3j$; $6l$ $4\times6m$	$1d$; $3k$ $2\times3k$; $6m$ $2\times6n$; $12o$	$2g$; $6n$ $4\times6l$ $4\times12o$
[p^2] $P\bar{6}m2$	p**a**, p**b**, **c**	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p}, \frac{v}{p}, 0)$ p = prime ≠ 3; $u, v = 1, \ldots, p-1$	$1a$; $(p-1)\times3j$; $\frac{(p-1)(p-2)}{6}\times6l$	$1b$; $(p-1)\times3k$; $\frac{(p-1)(p-2)}{6}\times6m$	$1c(e^*)$; $(p-1)\times3j$; $\frac{(p-1)(p-2)}{6}\times6l$ $2h(i^*)$; $(p-1)\times6n$; $\frac{(p-1)(p-2)}{6}\times12o$	$1d(f^*)$; $(p-1)\times3k$; $\frac{(p-1)(p-2)}{6}\times6m$ $2i(h^*)$; $(p-1)\times6n$; $\frac{(p-1)(p-2)}{6}\times12o$	$1e(c^*)$; $(p-1)\times3j$; $\frac{(p-1)(p-2)}{6}\times6l$ $p\times3j$; $\frac{p(p-1)}{2}\times6l$ $p^2\times6m$	$1f(d^*)$; $(p-1)\times3k$; $\frac{(p-1)(p-2)}{6}\times6m$ $p\times3k$; $\frac{p(p-1)}{2}\times6m$ $p\times6n$; $\frac{p(p-1)}{2}\times12o$	$2g$; $(p-1)\times6n$; $\frac{(p-1)(p-2)}{6}\times12o$ $p^2\times6l$ $p^2\times12o$

* $p = 3n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 187, pp. 668–669.

D_{3h}^{1} No. 187 $P\bar{6}m2$

	Axes	Coordinates	1a	1b	1c	1d	1e	1f	2g	2h 6l	2i 6m	3j 6n	3k 12o
I Maximal *translationengleiche* subgroups													
[2] $P\bar{6}$ (174)			1a	1b	1c	1d	1e	1f	2g	2h 2×3j	2i 2×3k	3j 6l	3k 2×6l
[2] $P3m1$ (156)			1a	1a	1b	1b	1c	1c	2×1a	2×1b 6e	2×1c 6e	3d 2×3d	3d 2×6e
[2] $P312$ (149)			1a	1b	1c	1d	1e	1f	2g	2h 6l	2i 6l	3j 6l	3k 2×6l
[3] $Cm2m$ (38)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	2a	2b	2a	2b	2a	2b	4c	4c 3×4d	4c 3×4e	2a; 4d 4c; 8f	2b; 4e 3×8f
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$											
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$											
$\widehat{=}$ $Amm2$	**c**, **a**, **a**+2**b**	$z, x-\frac{1}{2}y, \frac{1}{2}y$											
or	**c**, **b**, −2**a**−**b**	$z, -\frac{1}{2}x+y, -\frac{1}{2}x$											
or	**c**, −**a**−**b**, **a**−**b**	$z, \frac{1}{2}(x+y), \frac{1}{2}(x-y)$											
II Maximal *klassengleiche* subgroups													
Enlarged unit cell, non-isomorphic													
[2] $P\bar{6}c2$ (188)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	2a	2b	2c	2d	2e	2f	4g	4h 12l	4i 2×6k	6j 12l	6k 2×12l
[2] $P\bar{6}c2$ (188)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	2b	2a	2d	2c	2f	2e	4g	4h 2×6k	4i 12l	6k 12l	6j 2×12l
[3] $P\bar{6}2m$ (189)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y), \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	1a; 2c	1b; 2d	3f	3g	3f	3g	2e; 4h	6i 3×6j	6i 3×6k	3f; 6j 6i; 12l	3g; 6k 3×12l
[3] $P\bar{6}2m$ (189)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y)+\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	3f	3g	1a; 2c	1b; 2d	3f	3g	6i	2e; 4h 3×6j	6i 3×6k	3f; 6j 6i; 12l	3g; 6k 3×12l
[3] $P\bar{6}2m$ (189)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y)-\frac{1}{3}, \frac{1}{3}(-x+2y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	3f	3g	3f	3g	1a; 2c	1b; 2d	6i	6i 3×6j	2e; 4h 3×6k	3f; 6j 6i; 12l	3g; 6k 3×12l
Enlarged unit cell, isomorphic													
[2] $P\bar{6}m2$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	1a; 1b	2g	1c; 1d	2h	1e; 1f	2i	2×2g	2×2h 6l; 6m	2×2i 12o	3j; 3k 2×6n	6n 2×12o
[2] $P\bar{6}m2$	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	2g	1a; 1b	2h	1c; 1d	2i	1e; 1f	2×2g	2×2h 12o	2×2i 6l; 6m	6n 2×6n	3j; 3k 2×12o
[3] $P\bar{6}m2$	**a**, **b**, 3**c**	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	1a; 2g	1b; 2g	1c; 2h	1d; 2h	1e; 2i	1f; 2i	3×2g	3×2h 6l; 12o	3×2i 6m; 12o	3j; 6n 3×6n	3k; 6n 3×12o

Continued on preceding page

$P\bar{6}c2$ No. 188 D_{3h}^{2}

	Axes	Coordinates	Wyckoff positions					
			$2a$ $4g$	$2b$ $4h$	$2c$ $4i$	$2d$ $6j$	$2e$ $6k$	$2f$ $12l$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{6}$ (174)		$x,y,z+\frac{1}{4}$	$2g$ $2\times2g$	$1a;\,1b$ $2\times2h$	$2h$ $2\times2i$	$1c;\,1d$ $6l$	$2i$ $3j;\,3k$	$1e;1f$ $2\times6l$
[2] $P3c1$ (158)			$2a$ $2\times2a$	$2a$ $2\times2b$	$2b$ $2\times2c$	$2b$ $6d$	$2c$ $6d$	$2c$ $2\times6d$
[2] $P312$ (149)			$1a;\,1b$ $2\times2g$	$2g$ $2\times2h$	$1c;\,1d$ $2\times2i$	$2h$ $3j;\,3k$	$1e;\,1f$ $6l$	$2i$ $2\times6l$
[3] $C2cm$ (40)	$2\mathbf{a}+\mathbf{b},\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,-\frac{1}{2}x+y,z$	$4a$ $8c$	$4b$ $8c$	$4a$ $8c$	$4b$ $4a;\,8c$	$4a$ $3\times4b$	$4b$ $3\times8c$
conjugate:	$-\mathbf{a}+\mathbf{b},-\mathbf{a}-\mathbf{b},\mathbf{c}$	$\frac{1}{2}(-x+y),\frac{1}{2}(-x-y),z$						
conjugate:	$-\mathbf{a}-2\mathbf{b},\mathbf{a},\mathbf{c}$	$-\frac{1}{2}y,x-\frac{1}{2}y,z$						
$\widehat{=}\,Ama2$	$\mathbf{c},-\mathbf{b},2\mathbf{a}+\mathbf{b}$	$z,\frac{1}{2}x-y,\frac{1}{2}x$						
or	$\mathbf{c},\mathbf{a}+\mathbf{b},-\mathbf{a}+\mathbf{b}$	$z,\frac{1}{2}(x+y),\frac{1}{2}(-x+y)$						
or	$\mathbf{c},-\mathbf{a},-\mathbf{a}-2\mathbf{b}$	$z,-x+\frac{1}{2}y,-\frac{1}{2}y$						
alternative:								
$Cc2m$	$\mathbf{a},\mathbf{a}+2\mathbf{b},\mathbf{c}$	$x-\frac{1}{2}y,\frac{1}{2}y,z$						
or	$\mathbf{b},-2\mathbf{a}-\mathbf{b},\mathbf{c}$	$-\frac{1}{2}x+y,-\frac{1}{2}x,z$						
or	$-\mathbf{a}-\mathbf{b},\mathbf{a}-\mathbf{b},\mathbf{c}$	$-\frac{1}{2}(x+y),\frac{1}{2}(x-y),z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[3] $P\bar{6}2c$ (190)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+2\mathbf{b},\mathbf{c}$	$\frac{1}{3}(2x-y),\frac{1}{3}(x+y),z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4f$ $4e;2\times4f$	$2b;2c;2d$ $12i$	$6g$ $12i$	$6h$ $6g;12i$	$6g$ $3\times6h$	$6h$ $3\times12i$
[3] $P\bar{6}2c$ (190)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+2\mathbf{b},\mathbf{c}$	$\frac{1}{3}(2x-y)+\frac{1}{3},\frac{1}{3}(x+y),z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$6g$ $12i$	$6h$ $12i$	$6g$ $4e;2\times4f$	$6h$ $6g;12i$	$2a;4f$ $3\times6h$	$2b;2c;2d$ $3\times12i$
[3] $P\bar{6}2c$ (190)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+2\mathbf{b},\mathbf{c}$	$\frac{1}{3}(2x-y)-\frac{1}{3},\frac{1}{3}(x+y),z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$6g$ $12i$	$6h$ $4e;2\times4f$	$2a;4f$ $12i$	$2b;2c;2d$ $6g;12i$	$6g$ $3\times6h$	$6h$ $3\times12i$
Enlarged unit cell, isomorphic								
[3] $P\bar{6}c2$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z;\pm(0,0,\frac{1}{3})$	$2a;\,4g$ $3\times4g$	$2b;4g$ $3\times4h$	$2c;\,4h$ $3\times4i$	$2d;\,4h$ $6j;12l$	$2e;\,4i$ $6k;12l$	$2f;\,4i$ $3\times12l$
[p] $P\bar{6}c2$	$\mathbf{a},\mathbf{b},p\mathbf{c}$ $p=\text{prime}>2;\ u=1,\dots,p-1$	$x,y,\frac{1}{p}z;+(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4g$ $p\times4g$	$2b;\frac{p-1}{2}\times4g$ $p\times4h$	$2c;\frac{p-1}{2}\times4h$ $p\times4i$	$2d;\frac{p-1}{2}\times4h$ $6j;\frac{p-1}{2}\times12l$	$2e;\frac{p-1}{2}\times4i$ $6k;\frac{p-1}{2}\times12l$	$2f;\frac{p-1}{2}\times4i$ $p\times12l$
[4] $P\bar{6}c2$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z;+(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);+(\frac{1}{2},\frac{1}{2},0)$	$2a;\,6j$ $4g;12l$	$2b;6k$ $4i;12l$	$2e;\,6j$ $4h;12l$	$2f;\,6k$ $2\times6j;12l$	$2c;\,6j$ $4\times6k$	$2d;6k$ $4\times12l$
[p^2] $P\bar{6}c2$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$ $p=\text{prime}\neq3;\ u,v=1,\dots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z;+(\frac{u}{p},\frac{v}{p},0)$	$2a;(p-1)\times6j;$ $\frac{(p-1)(p-2)}{6}\times12l$ $4g;\frac{p^2-1}{3}\times12l$	$2b;\frac{p^2-1}{3}\times6k$ $4h(i^*);$ $\frac{p^2-1}{3}\times12l$	$2c(e^*);$ $(p-1)\times6j;$ $\frac{(p-1)(p-2)}{6}\times12l$ $4i(h^*);$ $\frac{p^2-1}{3}\times12l$	$2d(f^*);$ $\frac{p^2-1}{3}\times6k$ $p\times6j$ $\frac{p(p-1)}{2}\times12l$	$2e(c^*);$ $(p-1)\times6j;$ $\frac{(p-1)(p-2)}{6}\times12l$ $p^2\times6k$	$2f(d^*);$ $\frac{p^2-1}{3}\times6k$ $p^2\times12l$

$^*\,p=3n-1$

D_{3h}^3 No. 189 $P\bar{6}2m$

	Axes	Coordinates	Wyckoff positions					
			$1a$ $3g$	$1b$ $4h$	$2c$ $6i$	$2d$ $6j$	$2e$ $6k$	$3f$ $12l$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{6}$ (174)			$1a$ $3k$	$1b$ $2h$; $2i$	$1c$; $1e$ $6l$	$1d$; $1f$ $2\times3j$	$2g$ $2\times3k$	$3j$ $2\times6l$
[2] $P31m$ (157)			$1a$ $3c$	$1a$ $2\times2b$	$2b$ $2\times3c$	$2b$ $6d$	$2\times1a$ $6d$	$3c$ $2\times6d$
[2] $P321$ (150)			$1a$ $3f$	$1b$ $2\times2d$	$2d$ $6g$	$2d$ $6g$	$2c$ $6g$	$3e$ $2\times6g$
[3] $Cm2m$ (38)	$2\mathbf{a}+\mathbf{b}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, -\frac{1}{2}x+y, z$	$2a$ $2b$; $4e$	$2b$ $8f$	$4d$ $4c$; $8f$	$4e$ $3\times4d$	$4c$ $3\times4e$	$2a$; $4d$ $3\times8f$
conjugate:	$-\mathbf{a}+\mathbf{b}, -\mathbf{a}-\mathbf{b}, \mathbf{c}$	$\frac{1}{2}(-x+y), \frac{1}{2}(-x-y), z$						
conjugate:	$-\mathbf{a}-2\mathbf{b}, \mathbf{a}, \mathbf{c}$	$-\frac{1}{2}y, x-\frac{1}{2}y, z$						
$\widehat{=}$ $Amm2$	$\mathbf{c}, 2\mathbf{a}+\mathbf{b}, \mathbf{b}$	$z, \frac{1}{2}x, -\frac{1}{2}x+y$						
or	$\mathbf{c}, -\mathbf{a}+\mathbf{b}, -\mathbf{a}-\mathbf{b}$	$z, \frac{1}{2}(-x+y), \frac{1}{2}(-x-y)$						
or	$\mathbf{c}, -\mathbf{a}-2\mathbf{b}, \mathbf{a}$	$z, -\frac{1}{2}y, x-\frac{1}{2}y$						
alternative:								
$C2mm$	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$						
or	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$						
or	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $P\bar{6}2c$ (190)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$2a$ $6h$	$2b$ $2\times4f$	$4f$ $12i$	$2c$; $2d$ $12i$	$4e$ $2\times6h$	$6g$ $2\times12i$
[2] $P\bar{6}2c$ (190)	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$2b$ $6g$	$2a$ $2\times4f$	$2c$; $2d$ $12i$	$4f$ $2\times6h$	$4e$ $12i$	$6h$ $2\times12i$
[3] $P\bar{6}m2$ (187)	$\mathbf{a}-\mathbf{b}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(2x-y), \frac{1}{3}(x+y), z;$ $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a$; $1c$; $1e$ $3\times3k$	$1b$; $1d$; $1f$ $12o$	$6l$ $3\times6n$	$6m$ $3\times6l$	$2g$; $2h$; $2i$ $3\times6m$	$3\times3j$ $3\times12o$
Enlarged unit cell, isomorphic								
[2] $P\bar{6}2m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z; +(0,0,\frac{1}{2})$	$1a$; $1b$ $6i$	$2e$ $2\times4h$	$2c$; $2d$ $2\times6i$	$4h$ $6j$; $6k$	$2\times2e$ $12l$	$3f$; $3g$ $2\times12l$
[2] $P\bar{6}2m$	$\mathbf{a}, \mathbf{b}, 2\mathbf{c}$	$x, y, \frac{1}{2}z+\frac{1}{4}; +(0,0,\frac{1}{2})$	$2e$ $3f$; $3g$	$1a$; $1b$ $2\times4h$	$4h$ $2\times6i$	$2c$; $2d$ $12l$	$2\times2e$ $6j$; $6k$	$6i$ $2\times12l$
[3] $P\bar{6}2m$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x, y, \frac{1}{3}z; \pm(0,0,\frac{1}{3})$	$1a$; $2e$ $3g$; $6i$	$1b$; $2e$ $3\times4h$	$2c$; $4h$ $3\times6i$	$2d$; $4h$ $6j$; $12l$	$3\times2e$ $6k$; $12l$	$3f$; $6i$ $3\times12l$
[p] $P\bar{6}2m$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x, y, \frac{1}{p}z; +(0,0,\frac{u}{p})$ $p = \text{prime} > 2$; $u = 1,\ldots,p-1$	$1a$; $\frac{p-1}{2}\times2e$ $3g$; $\frac{p-1}{2}\times6i$	$1b$; $\frac{p-1}{2}\times2e$ $p\times4h$	$2c$; $\frac{p-1}{2}\times4h$ $p\times6i$	$2d$; $\frac{p-1}{2}\times4h$ $6j$; $\frac{p-1}{2}\times12l$	$p\times2e$ $6k$; $\frac{p-1}{2}\times12l$	$3f$; $\frac{p-1}{2}\times6i$ $p\times12l$
[4] $P\bar{6}2m$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z; +(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0); +(\frac{1}{2},\frac{1}{2},0)$	$1a$; $3f$ $2\times3g$; $6k$	$1b$; $3g$ $4h$; $12l$	$2c$; $6j$ $2\times6i$; $12l$	$2d$; $6k$ $4\times6j$	$2e$; $6i$ $4\times6k$	$2\times3f$; $6j$ $4\times12l$
[p^2] $P\bar{6}2m$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z; +(\frac{u}{p},\frac{v}{p},0)$ $p = \text{prime} \neq 3$; $u, v = 1,\ldots,p-1$	$1a$; $(p-1)\times3f$; $\frac{(p-1)(p-2)}{6}\times6j$ $p\times3g$; $\frac{p(p-1)}{2}\times6k$	$1b$; $(p-1)\times3g$; $\frac{(p-1)(p-2)}{6}\times6k$ $4h$; $\frac{p^2-1}{3}\times12l$	$2c$; $\frac{p^2-1}{3}\times6j$ $p\times6i$; $\frac{p(p-1)}{2}\times12l$	$2d$; $\frac{p^2-1}{3}\times6k$ $p^2\times6j$	$2e$; $(p-1)\times6i$; $\frac{(p-1)(p-2)}{6}\times12l$ $p^2\times6k$	$p\times3f$; $\frac{p(p-1)}{2}\times6j$ $p^2\times12l$

$P\bar{6}2c$ No. 190 D_{3h}^{4}

	Axes	Coordinates	Wyckoff positions $2a$	$2b$	$2c$	$2d$ $6g$	$4e$ $6h$	$4f$ $12i$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{6}$ (174)		$x,y,z+\frac{1}{4}$	$2g$	$1a$; $1b$	$1d$; $1e$	$1c$; $1f$ $6l$	$2\times 2g$ $3j$; $3k$	$2h$; $2i$ $2\times 6l$
[2] $P31c$ (159)			$2a$	$2a$	$2b$	$2b$ $6c$	$2\times 2a$ $6c$	$2\times 2b$ $2\times 6c$
[2] $P321$ (150)			$1a$; $1b$	$2c$	$2d$	$2d$ $3e$; $3f$	$2\times 2c$ $6g$	$2\times 2d$ $2\times 6g$
[3] $C2cm$ (40)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y,\frac{1}{2}y,z$	$4a$	$4b$	$4b$	$4b$ $4a$; $8c$	$8c$ $3\times 4b$	$8c$ $3\times 8c$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y,-\frac{1}{2}x,z$						
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y),\frac{1}{2}(x-y),z$						
$\widehat{=}$ $Ama2$	**c**, **a**+2**b**, −**a**	$z,\frac{1}{2}y,-x+\frac{1}{2}y$						
or	**c**, −2**a**−**b**, −**b**	$z,-\frac{1}{2}x,\frac{1}{2}x-y$						
or	**c**, **a**−**b**, **a**+**b**	$z,\frac{1}{2}(x-y),\frac{1}{2}(x+y)$						
alternative:								
$Cc2m$	2**a**+**b**, **b**, **c**	$\frac{1}{2}x,-\frac{1}{2}x+y,z$						
or	−**a**−2**b**, **a**, **c**	$-\frac{1}{2}y,x-\frac{1}{2}y,z$						
or	−**a**+**b**, −**a**−**b**, **c**	$\frac{1}{2}(-x+y),\frac{1}{2}(-x-y),z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[3] $P\bar{6}c2$ (188)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y),z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a$; $2c$; $2e$	$2b$; $2d$; $2f$	$6k$	$6k$ $3\times 6j$	$4g$; $4h$; $4i$ $3\times 6k$	$12l$ $3\times 12l$
Enlarged unit cell, isomorphic								
[3] $P\bar{6}2c$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$	$2b$; $4e$	$2d$; $4f$	$2c$; $4f$ $6g$; $12i$	$3\times 4e$ $6h$; $12i$	$3\times 4f$ $3\times 12i$
[p] $P\bar{6}2c$	**a**, **b**, p**c** p = prime > 2; $u=1,\ldots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times 4e$	$2b$; $\frac{p-1}{2}\times 4e$	$2c(d^{*})$; $\frac{p-1}{2}\times 4f$	$2d(c^{*})$; $\frac{p-1}{2}\times 4f$ $6g$; $\frac{p-1}{2}\times 12i$	$p\times 4e$ $6h$; $\frac{p-1}{2}\times 12i$	$p\times 4f$ $p\times 12i$
[4] $P\bar{6}2c$	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6g$	$2b$; $6h$	$2d$; $6h$	$2c$; $6h$ $2\times 6g$; $12i$	$4e$; $12i$ $4\times 6h$	$4f$; $12i$ $4\times 12i$
[p^2] $P\bar{6}2c$	p**a**, p**b**, **c** p = prime ≠ 3; $u,v=1,\ldots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a$; $(p-1)\times 6g$; $\frac{(p-1)(p-2)}{6}\times 12i$	$2b$; $\frac{p^2-1}{3}\times 6h$	$2c(d^{\dagger})$; $\frac{p^2-1}{3}\times 6h$	$2d(c^{\dagger})$; $\frac{p^2-1}{3}\times 6h$ $p\times 6g$; $\frac{p(p-1)}{2}\times 12i$	$4e$; $\frac{p^2-1}{3}\times 12i$ $p^2\times 6h$	$4f$; $\frac{p^2-1}{3}\times 12i$ $p^2\times 12i$

* $p=4n-1$ † $p=3n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 191, pp. 673–674.

D^1_{6h} $P6/m2/m2/m$ No. 191 $P6/mmm$

	Axes	Coordinates	Wyckoff positions 1*a*	1*b*	2*c*	2*d*	2*e*	3*f*	3*g*	4*h*	6*i* 12*n*	6*j* 12*o*	6*k* 12*p*	6*l* 12*q*	6*m* 24*r*
I Maximal *translationengleiche* subgroups															
[2] $P\bar{6}2m$ (189)			1*a*	1*b*	2*c*	2*d*	2*e*	3*f*	3*g*	4*h*	6*i* 2×6*i*	2×3*f* 12*l*	2×3*g* 2×6*j*	6*j* 2×6*k*	6*k* 2×12*l*
[2] $P\bar{6}m2$ (187)			1*a*	1*b*	1*c*; 1*e*	1*d*; 1*f*	2*g*	3*j*	3*k*	2*h*; 2*i*	6*n* 12*o*	6*l* 2×6*n*	6*m* 2×6*l*	2×3*j* 2×6*m*	2×3*k* 2×12*o*
[2] $P6mm$ (183)			1*a*	1*a*	2*b*	2*b*	2×1*a*	3*c*	3*c*	2×2*b*	2×3*c* 2×6*d*	6*d* 2×6*e*	6*d* 12*f*	6*e* 12*f*	6*e* 2×12*f*
[2] $P622$ (177)			1*a*	1*b*	2*c*	2*d*	2*e*	3*f*	3*g*	4*h*	6*i* 12*n*	6*j* 12*n*	6*k* 12*n*	6*l* 12*n*	6*m* 2×12*n*
[2] $P6/m$ (175)			1*a*	1*b*	2*c*	2*d*	2*e*	3*f*	3*g*	4*h*	6*i* 12*l*	6*j* 12*l*	6*k* 2×6*j*	6*j* 2×6*k*	6*k* 2×12*l*
[2] $P\bar{3}m1$ (164)			1*a*	1*b*	2*d*	2*d*	2*c*	3*e*	3*f*	2×2*d*	6*i* 12*j*	6*g* 2×6*i*	6*h* 12*j*	6*i* 12*j*	6*i* 2×12*j*
[2] $P\bar{3}1m$ (162)			1*a*	1*b*	2*c*	2*d*	2*e*	3*f*	3*g*	4*h*	6*k* 2×6*k*	6*k* 12*l*	6*k* 12*l*	6*i* 12*l*	6*j* 2×12*l*
[3] $Cmmm$ (65)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y, \frac{1}{2}y, z$	2*a*	2*d*	4*i*	4*j*	4*k*	2*b*; 4*e*	2*c*; 4*f*	8*n*	4*l*; 8*m* 8*o*; 16*r*	4*g*; 8*p* 8*n*; 16*r*	4*h*; 8*q* 3×8*p*	4*i*; 8*p* 3×8*q*	4*j*; 8*q* 3×16*r*
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$													
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$													
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**															
[2] $P6_3/mmc$ (194)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*a*	2*b*	4*f*	2*c*; 2*d*	4*e*	6*g*	6*h*	2×4*f*	12*k* 24*l*	12*i* 2×12*k*	12*j* 24*l*	12*k* 2×12*j*	2×6*h* 2×24*l*
[2] $P6_3/mmc$ (194)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*b*	2*a*	2*c*; 2*d*	4*f*	4*e*	6*h*	6*g*	2×4*f*	12*k* 24*l*	12*j* 2×12*k*	12*i* 2×12*j*	2×6*h* 24*l*	12*k* 2×24*l*
[2] $P6_3/mcm$ (193)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*b*	2*a*	4*d*	4*c*	4*e*	6*f*	6*g*	8*h*	12*k* 2×12*k*	12*k* 24*l*	2×6*g* 24*l*	12*i* 2×12*j*	12*j* 2×24*l*
[2] $P6_3/mcm$ (193)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*a*	2*b*	4*c*	4*d*	4*e*	6*g*	6*f*	8*h*	12*k* 2×12*k*	2×6*g* 24*l*	12*k* 2×12*j*	12*j* 24*l*	12*i* 2×24*l*
[2] $P6/mcc$ (192)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z$; $+(0,0,\frac{1}{2})$	2*b*	2*a*	4*d*	4*c*	4*e*	6*g*	6*f*	8*h*	12*i* 24*m*	12*l* 24*m*	12*j* 2×12*l*	12*l* 24*m*	12*k* 2×24*m*
[2] $P6/mcc$ (192)	**a**, **b**, 2**c**	$x, y, \frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	2*a*	2*b*	4*c*	4*d*	4*e*	6*f*	6*g*	8*h*	12*i* 24*m*	12*j* 24*m*	12*l* 24*m*	12*k* 2×12*l*	12*l* 2×24*m*

	Axes	Coordinates	Wyckoff positions						
			$1a$	$1b$ $4h$	$2c$ $6i$ $12n$	$2d$ $6j$ $12o$	$2e$ $6k$ $12p$	$3f$ $6l$ $12q$	$3g$ $6m$ $24r$
Enlarged unit cell, isomorphic									
[2] $P6/mmm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z$; $+(0,0,\frac{1}{2})$	$1a;1b$	$2e$ $2\times4h$	$2c;2d$ $2\times6i$ $2\times12n$	$4h$ $6j;6k$ $2\times12o$	$2\times2e$ $12n$ $12p;12q$	$3f;3g$ $6l;6m$ $24r$	$6i$ $12o$ $2\times24r$
[2] $P6/mmm$	$\mathbf{a},\mathbf{b},2\mathbf{c}$	$x,y,\frac{1}{2}z+\frac{1}{4}$; $+(0,0,\frac{1}{2})$	$2e$	$1a;1b$ $2\times4h$	$4h$ $2\times6i$ $2\times12n$	$2c;2d$ $12n$ $2\times12o$	$2\times2e$ $6j;6k$ $24r$	$6i$ $12o$ $12p;12q$	$3f;3g$ $6l;6m$ $2\times24r$
[3] $P6/mmm$	$\mathbf{a},\mathbf{b},3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$1a;2e$	$1b;2e$ $3\times4h$	$2c;4h$ $3\times6i$ $3\times12n$	$2d;4h$ $6j;12n$ $3\times12o$	$3\times2e$ $6k;12n$ $12p;24r$	$3f;6i$ $6l;12o$ $12q;24r$	$3g;6i$ $6m;12o$ $3\times24r$
[p] $P6/mmm$	$\mathbf{a},\mathbf{b},p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $p=\text{prime}>2;\ u=1,\ldots,p-1$	$1a;\frac{p-1}{2}\times2e$	$1b;\frac{p-1}{2}\times2e$ $p\times4h$	$2c;\frac{p-1}{2}\times4h$ $p\times6i$ $p\times12n$	$2d;\frac{p-1}{2}\times4h$ $6j;\frac{p-1}{2}\times12n$ $p\times12o$	$p\times2e$ $6k;\frac{p-1}{2}\times12n$ $12p;\frac{p-1}{2}\times24r$	$3f;\frac{p-1}{2}\times6i$ $6l;\frac{p-1}{2}\times12o$ $12q;\frac{p-1}{2}\times24r$	$3g;\frac{p-1}{2}\times6i$ $6m;\frac{p-1}{2}\times12o$ $p\times24r$
[3] $P6/mmm$	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b},\ \mathbf{c}$	$\frac{1}{3}(x+y)$, $\frac{1}{3}(-x+2y),z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$1a;2c$	$1b;2d$ $12n$	$6j$ $6i;12o$ $3\times12o$	$6k$ $3\times6l$ $12n;24r$	$2e;4h$ $3\times6m$ $3\times12p$	$3f;6l$ $6j;12p$ $3\times12q$	$3g;6m$ $6k;12q$ $3\times24r$
[4] $P6/mmm$	$2\mathbf{a},2\mathbf{b},\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0);+(\frac{1}{2},\frac{1}{2},0)$	$1a;3f$	$1b;3g$ $4h;12o$	$2c;6l$ $12n;12o$ $2\times12n;24r$	$2d;6m$ $2\times6j;12p$ $2\times12o;24r$	$2e;6i$ $2\times6k;12q$ $4\times12p$	$6j;6l$ $2\times6l;12p$ $4\times12q$	$6k;6m$ $2\times6m;12q$ $4\times24r$
[p^2] $P6/mmm$	$p\mathbf{a},p\mathbf{b},\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$ $p=\text{prime}>4$; $u,v=1,\ldots,p-1$	$1a;\frac{p-1}{2}\times6j$; $\frac{p-1}{2}\times6l$; $\frac{(p-1)(p-5)}{12}\times12p$	$1b;\frac{p-1}{2}\times6k$; $\frac{p-1}{2}\times6m$; $\frac{(p-1)(p-5)}{12}\times12p$ $4h$; $(p-1)\times12o$; $\frac{(p-1)(p-2)}{6}\times24r$	$2c$; $(p-1)\times6l$; $\frac{(p-1)(p-2)}{6}\times12p$ $6i;\frac{p-1}{2}\times12n$; $\frac{p-1}{2}\times12o$; $\frac{(p-1)^2}{4}\times24r$ $p\times12n$; $\frac{p(p-1)}{2}\times24r$	$2d$; $(p-1)\times6m$; $\frac{(p-1)(p-2)}{6}\times12p$ $p\times6j$; $\frac{p(p-1)}{2}\times12p$ $p\times12o$; $\frac{p(p-1)}{2}\times24r$	$2e;\frac{p-1}{2}\times12n$; $\frac{p-1}{2}\times12o$; $\frac{(p-1)(p-5)}{12}\times24r$ $p\times6k$; $\frac{p(p-1)}{2}\times12q$ $p^2\times12p$	$3f;\frac{p-1}{2}\times6j$; $\frac{p-1}{2}\times6l$; $\frac{(p-1)^2}{4}\times12p$ $p\times6l$; $\frac{p(p-1)}{2}\times12p$ $p^2\times12q$	$3g;\frac{p-1}{2}\times6k$ $\frac{p-1}{2}\times6m$; $\frac{(p-1)^2}{4}\times12q$ $p\times6m$; $\frac{p(p-1)}{2}\times12q$ $p^2\times24r$

D_{6h}^2 $\quad P6/m2/c2/c$ $\quad$ No. 192 $\quad P6/mcc$

	Axes	Coordinates	Wyckoff positions $2a$	 $2b$ $8h$	 $4c$ $12i$	 $4d$ $12j$	 $4e$ $12k$	 $6f$ $12l$	 $6g$ $24m$
I Maximal *translationengleiche* subgroups									
[2] $P\bar{6}2c$ (190)		$x,y,z+\frac{1}{4}$	$2a$	$2b$ $2\times4f$	$4f$ $12i$	$2c;2d$ $2\times6g$	$4e$ $12i$	$6g$ $2\times6h$	$6h$ $2\times12i$
[2] $P\bar{6}c2$ (188)		$x,y,z+\frac{1}{4}$	$2a$	$2b$ $4h;4i$	$2c;2e$ $12l$	$2d;2f$ $12l$	$4g$ $2\times6j$	$6j$ $2\times6k$	$6k$ $2\times12l$
[2] $P6cc$ (184)			$2a$	$2a$ $2\times4b$	$4b$ $2\times6c$	$4b$ $12d$	$2\times2a$ $12d$	$6c$ $12d$	$6c$ $2\times12d$
[2] $P622$ (177)		$x,y,z+\frac{1}{4}$	$1a;1b$	$2e$ $2\times4h$	$2c;2d$ $2\times6i$	$4h$ $6j;6k$	$2\times2e$ $6l;6m$	$3f;3g$ $12n$	$6i$ $2\times12n$
[2] $P6/m$ (175)			$2e$	$1a;1b$ $2\times4h$	$4h$ $2\times6i$	$2c;2d$ $12l$	$2\times2e$ $12l$	$6i$ $6j;6k$	$3f;3g$ $2\times12l$
[2] $P\bar{3}c1$ (165)			$2a$	$2b$ $2\times4d$	$4d$ $12g$	$4d$ $2\times6f$	$4c$ $12g$	$6f$ $12g$	$6e$ $2\times12g$
[2] $P\bar{3}1c$ (163)			$2a$	$2b$ $2\times4f$	$2c;2d$ $12i$	$4f$ $12i$	$4e$ $2\times6h$	$6h$ $12i$	$6g$ $2\times12i$
[3] $Cccm$ (66)	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	$x-\frac{1}{2}y, \frac{1}{2}y, z$	$4a$	$4c$ $16m$	$8h$ $8j;2\times8k$	$8l$ $8g;16m$	$8i$ $8h;16m$	$4b;8k$ $3\times8l$	$4d;4e;4f$ $3\times16m$
conjugate:	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}x+y, -\frac{1}{2}x, z$							
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	$-\frac{1}{2}(x+y), \frac{1}{2}(x-y), z$							
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**									
[3] $P6/mcc$	$\mathbf{a}, \mathbf{b}, 3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a;4e$	$2b;4e$ $3\times8h$	$4c;8h$ $3\times12i$	$4d;8h$ $12j;24m$	$3\times4e$ $12k;24m$	$6f;12i$ $12l;24m$	$6g;12i$ $3\times24m$
[p] $P6/mcc$ $p=\text{prime}>2; u=1,\ldots,p-1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a;\frac{p-1}{2}\times4e$	$2b;\frac{p-1}{2}\times4e$ $p\times8h$	$4c;\frac{p-1}{2}\times8h$ $p\times12i$	$4d;\frac{p-1}{2}\times8h$ $12j$; $\frac{p-1}{2}\times24m$	$p\times4e$ $12k$; $\frac{p-1}{2}\times24m$	$6f;\frac{p-1}{2}\times12i$ $12l$; $\frac{p-1}{2}\times24m$	$6g;\frac{p-1}{2}\times12i$ $p\times24m$
[3] $P6/mcc$	$2\mathbf{a}+\mathbf{b}$, $-\mathbf{a}+\mathbf{b}, \mathbf{c}$	$\frac{1}{3}(x+y)$, $\frac{1}{3}(-x+2y), z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2a;4c$	$2b;4d$ $24m$	$12j$ $12i;24m$	$12l$ $3\times12k$	$4e;8h$ $12j;24m$	$6f;12k$ $3\times12l$	$6g;12l$ $3\times24m$
[4] $P6/mcc$	$2\mathbf{a}, 2\mathbf{b}, \mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a;6f$	$2b;6g$ $8h;24m$	$4c;12k$ $2\times24m$	$4d;12l$ $2\times12j;24m$	$4e;12i$ $2\times12k;24m$	$12j;12k$ $4\times12l$	$2\times12l$ $4\times24m$
[p^2] $P6/mcc$ $p=\text{prime}>4$; $u,v=1,\ldots,p-1$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a;\frac{p-1}{2}\times12j$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)(p-5)}{12}\times$ $24m$	$2b$; $\frac{p^2-1}{6}\times12l$ $8h$; $\frac{p^2-1}{3}\times24m$	$4c$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times$ $24m$ $12i$; $\frac{p^2-1}{2}\times24m$	$4d$; $\frac{p^2-1}{3}\times12l$ $p\times12j$; $\frac{p(p-1)}{2}\times$ $24m$	$4e$; $\frac{p^2-1}{6}\times24m$ $p\times12k$; $\frac{p(p-1)}{2}\times$ $24m$	$6f$; $\frac{p-1}{2}\times12j$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)^2}{4}\times24m$ $p^2\times12l$	$6g$; $\frac{p^2-1}{2}\times12l$ $p^2\times24m$

$P6_3/mcm$ No. 193 $P6_3/m2/c2/m$ D_{6h}^3

	Axes	Coordinates	Wyckoff positions					
			$2a$ $6g$	$2b$ $8h$	$4c$ $12i$	$4d$ $12j$	$4e$ $12k$	$6f$ $24l$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{6}2m$ (189)		$x,y,z+\frac{1}{4}$	$1a$; $1b$ $3f$; $3g$	$2e$ $2\times4h$	$2c$; $2d$ $12l$	$4h$ $6j$; $6k$	$2\times2e$ $2\times6i$	$6i$ $2\times12l$
[2] $P\bar{6}c2$ (188)			$2b$ $6k$	$2a$ $4h$; $4i$	$2d$; $2f$ $2\times6j$	$2c$; $2e$ $2\times6k$	$4g$ $12l$	$6j$ $2\times12l$
[2] $P6_3cm$ (185)			$2a$ $6c$	$2a$ $2\times4b$	$4b$ $12d$	$4b$ $12d$	$2\times2a$ $2\times6c$	$6c$ $2\times12d$
[2] $P6_322$ (182)		$x,y,z+\frac{1}{4}$	$2a$ $6g$	$2b$ $2\times4f$	$4f$ $2\times6h$	$2c$; $2d$ $12i$	$4e$ $12i$	$6h$ $2\times12i$
[2] $P6_3/m$ (176)			$2a$ $6h$	$2b$ $2\times4f$	$2c$; $2d$ $12i$	$4f$ $2\times6h$	$4e$ $12i$	$6g$ $2\times12i$
[2] $P\bar{3}c1$ (165)			$2a$ $6f$	$2b$ $2\times4d$	$4d$ $12g$	$4d$ $12g$	$4c$ $12g$	$6e$ $2\times12g$
[2] $P\bar{3}1m$ (162)			$2e$ $6k$	$1a$; $1b$ $2\times4h$	$4h$ $6i$; $6j$	$2c$; $2d$ $12l$	$2\times2e$ $2\times6k$	$3f$; $3g$ $2\times12l$
[3] $Cmcm$ (63)	$2\mathbf{a}+\mathbf{b}$, $\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x,-\frac{1}{2}x+y,z$	$4c$ $4c$; $8g$	$4a$ $16h$	$8g$ $8e$; $16h$	$8e$ $3\times8g$	$8f$ $8f$; $16h$	$4b$; $8d$ $3\times16h$
conjugate:	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{a}-\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}(-x+y),-\frac{1}{2}(x+y),z$						
conjugate:	$-\mathbf{a}-2\mathbf{b}$, $\mathbf{a}$, $\mathbf{c}$	$-\frac{1}{2}y,x-\frac{1}{2}y,z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[3] $P6_3/mmc$ (194)	$\mathbf{a}-\mathbf{b}$, $\mathbf{a}+2\mathbf{b}$, $\mathbf{c}$	$\frac{1}{3}(2x-y),\frac{1}{3}(x+y),z$; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2b$; $2c$; $2d$ $3\times6h$	$2a$; $4f$ $24l$	$12j$ $12i$; $24l$	$12i$ $3\times12j$	$4e$; $2\times4f$ $3\times12k$	$6g$; $12k$ $3\times24l$
Enlarged unit cell, isomorphic								
[3] $P6_3/mcm$	$\mathbf{a}$, $\mathbf{b}$, $3\mathbf{c}$	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$ $6g$; $12k$	$2b$; $4e$ $3\times8h$	$4c$; $8h$ $12i$; $24l$	$4d$; $8h$ $12j$; $24l$	$3\times4e$ $3\times12k$	$6f$; $12k$ $3\times24l$
[p] $P6_3/mcm$	$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$ $p=$ prime >2; $u=1,\dots,p-1$	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$	$2a$; $\frac{p-1}{2}\times4e$ $6g$; $\frac{p-1}{2}\times12k$	$2b$; $\frac{p-1}{2}\times4e$ $p\times8h$	$4c$; $\frac{p-1}{2}\times8h$ $12i$; $\frac{p-1}{2}\times24l$	$4d$; $\frac{p-1}{2}\times8h$ $12j$; $\frac{p-1}{2}\times24l$	$p\times4e$ $p\times12k$	$6f$; $\frac{p-1}{2}\times12k$ $p\times24l$
[4] $P6_3/mcm$	$2\mathbf{a}$, $2\mathbf{b}$, $\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6g$ $2\times6g$; $12j$	$2b$; $6f$ $8h$; $24l$	$4c$; $12j$ $2\times12i$; $24l$	$4d$; $12i$ $4\times12j$	$4e$; $12k$ $2\times12k$; $24l$	$12i$; $12k$ $4\times24l$
[p^2] $P6_3/mcm$	$p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ $p=$ prime >4; $u,v=1,\dots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$	$2a$; $(p-1)\times6g$; $\frac{(p-1)(p-2)}{6}\times12j$	$2b$; $\frac{p-1}{2}\times12i$ $\frac{p-1}{2}\times12k$; $\frac{(p-1)(p-5)}{12}\times24l$	$4c$; $\frac{p^2-1}{3}\times12j$	$4d$; $(p-1)\times12i$; $\frac{(p-1)(p-2)}{6}\times24l$	$4e$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times24l$	$6f$; $\frac{p-1}{2}\times12i$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)^2}{4}\times24l$
			$p\times6g$; $\frac{p(p-1)}{2}\times12j$	$8h$; $\frac{p^2-1}{3}\times24l$	$p\times12i$; $\frac{p(p-1)}{2}\times24l$	$p^2\times12j$	$p\times12k$; $\frac{p(p-1)}{2}\times24l$	$p^2\times24l$

D_{6h}^4 $\quad P6_3/m2/m2/c$ $\quad$ No. 194 $\quad P6_3/mmc$

	Axes	Coordinates	Wyckoff positions					
			$2a$ $6g$	$2b$ $6h$	$2c$ $12i$	$2d$ $12j$	$4e$ $12k$	$4f$ $24l$
I Maximal *translationengleiche* subgroups								
[2] $P\bar{6}2c$ (190)			$2a$ $6g$	$2b$ $6h$	$2c$ $2\times6g$	$2d$ $2\times6h$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P\bar{6}m2$ (187)		$x,y,z+\frac{1}{4}$	$2g$ $6n$	$1a$; $1b$ $3j$; $3k$	$1d$; $1e$ $12o$	$1c$; $1f$ $6l$; $6m$	$2\times2g$ $2\times6n$	$2h$; $2i$ $2\times12o$
[2] $P6_3mc$ (186)			$2a$ $6c$	$2a$ $6c$	$2b$ $12d$	$2b$ $12d$	$2\times2a$ $2\times6c$	$2\times2b$ $2\times12d$
[2] $P6_322$ (182)			$2a$ $6g$	$2b$ $6h$	$2c$ $2\times6g$	$2d$ $12i$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P6_3/m$ (176)			$2b$ $6g$	$2a$ $6h$	$2c$ $12i$	$2d$ $2\times6h$	$4e$ $12i$	$4f$ $2\times12i$
[2] $P\bar{3}m1$ (164)			$1a$; $1b$ $3e$; $3f$	$2c$ $6i$	$2d$ $6g$; $6h$	$2d$ $12j$	$2\times2c$ $2\times6i$	$2\times2d$ $2\times12j$
[2] $P\bar{3}1c$ (163)			$2b$ $6g$	$2a$ $6h$	$2c$ $12i$	$2d$ $12i$	$4e$ $12i$	$4f$ $2\times12i$
[3] $Cmcm$ (63)	**a**, **a**+2**b**, **c**	$x-\frac{1}{2}y,\frac{1}{2}y,z$	$4a$ $4b$; $8d$	$4c$ $4c$; $8g$	$4c$ $8e$; $16h$	$4c$ $3\times8g$	$8f$ $8f$; $16h$	$8f$ $3\times16h$
conjugate:	**b**, −2**a**−**b**, **c**	$-\frac{1}{2}x+y,-\frac{1}{2}x,z$						
conjugate:	−**a**−**b**, **a**−**b**, **c**	$-\frac{1}{2}(x+y),\frac{1}{2}(x-y),z$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[3] $P6_3/mcm$ (193)	2**a**+**b**, −**a**+**b**, **c**	$\frac{1}{3}(x+y),\frac{1}{3}(-x+2y)$, z; $\pm(\frac{1}{3},\frac{2}{3},0)$	$2b$; $4d$ $6f$; $12i$	$2a$; $4c$ $6g$; $12j$	$6g$ $3\times12i$	$6g$ $3\times12j$	$4e$; $8h$ $12k$; $24l$	$12k$ $3\times24l$
Enlarged unit cell, isomorphic								
[3] $P6_3/mmc$	**a**, **b**, 3**c**	$x,y,\frac{1}{3}z$; $\pm(0,0,\frac{1}{3})$	$2a$; $4e$ $6g$; $12k$	$2b$; $4e$ $6h$; $12k$	$2d$; $4f$ $12i$; $24l$	$2c$; $4f$ $12j$; $24l$	$3\times4e$ $3\times12k$	$3\times4f$ $3\times24l$
[p] $P6_3/mmc$	**a**, **b**, p**c** $p=$ prime >2;	$x,y,\frac{1}{p}z$; $+(0,0,\frac{u}{p})$ $u=1\ldots p-1$	$2a$; $\frac{p-1}{2}\times4e$ $6g$; $\frac{p-1}{2}\times12k$	$2b$; $\frac{p-1}{2}\times4e$ $6h$; $\frac{p-1}{2}\times12k$	$2c(d^*)$; $\frac{p-1}{2}\times4f$ $12i$; $\frac{p-1}{2}\times24l$	$2d(c^*)$; $\frac{p-1}{2}\times4f$ $12j$; $\frac{p-1}{2}\times24l$	$p\times4e$ $p\times12k$	$p\times4f$ $p\times24l$
[4] $P6_3/mmc$	2**a**, 2**b**, **c**	$\frac{1}{2}x,\frac{1}{2}y,z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(\frac{1}{2},\frac{1}{2},0)$	$2a$; $6g$ $12i$; $12k$	$2b$; $6h$ $2\times6h$; $12j$	$2d$; $6h$ $2\times12i$; $24l$	$2c$; $6h$ $4\times12j$	$4e$; $12k$ $2\times12k$; $24l$	$4f$; $12k$ $4\times24l$
[p^2] $P6_3/mmc$	p**a**, p**b**, **c** $p=$ prime >4;	$\frac{1}{p}x,\frac{1}{p}y,z$; $+(\frac{u}{p},\frac{v}{p},0)$ $u,v=1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times12i$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)(p-5)}{12}\times24l$ $6g$; $\frac{p-1}{2}\times12i$; $\frac{p-1}{2}\times12k$; $\frac{(p-1)^2}{4}\times24l$	$2b$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p\times6h$; $\frac{p(p-1)}{2}\times12j$	$2c(d^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p\times12i$; $\frac{p(p-1)}{2}\times24l$	$2d(c^\dagger)$; $(p-1)\times6h$; $\frac{(p-1)(p-2)}{6}\times12j$ $p^2\times12j$	$4e$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times24l$ $p\times12k$; $\frac{p(p-1)}{2}\times24l$	$4f$; $(p-1)\times12k$; $\frac{(p-1)(p-2)}{6}\times24l$ $p^2\times24l$

* $p=4n-1$ $\quad$ † $p=6n-1$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 195, pp. 678–679.

$P23$ No. 195 T^1

	Axes	Coordinates	Wyckoff positions						
			$1a$	$1b$	$3c$	$3d$	$4e$ $6h$	$6f$ $6i$	$6g$ $12j$
I Maximal *translationengleiche* subgroups									
[4] $R3$ (146)	(rhombohedral axes)		$1a$	$1a$	$3b$	$3b$	$1a;3b$ $2\times3b$	$2\times3b$ $2\times3b$	$2\times3b$ $4\times3b$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y-z), \frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$3a$	$3a$	$9b$	$9b$	$3a;9b$ $2\times9b$	$2\times9b$ $2\times9b$	$2\times9b$ $4\times9b$
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z), \frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)$							
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $-\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z), \frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)$							
	conjugate: $-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z), \frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$							
[3] $P222$ (16)			$1a$	$1h$	$1e;1f;1g$	$1b;1c;1d$	$4u$ $2k;2n;2r$	$2i;2m;2q$ $2l;2p;2t$	$2j;2o;2s$ $3\times4u$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**									
[2] $F23$ (196)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$4a;4b$	$4c;4d$	$24g$	$24f$	$2\times16e$ $48h$	$2\times24f$ $2\times24g$	$48h$ $2\times48h$
[4] $I2_13$ (199)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$8a$	$8a$	$2\times12b$	$2\times12b$	$8a;24c$ $2\times24c$	$2\times24c$ $2\times24c$	$4\times12b$ $4\times24c$
[4] $I2_13$ (199)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$8a$	$8a$	$2\times12b$	$2\times12b$	$8a;24c$ $4\times12b$	$2\times24c$ $2\times24c$	$2\times24c$ $4\times24c$
[4] $I23$ (197)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$2a;6b$	$8c$	$24f$	$12d;12e$	$8c;24f$ $2\times24f$	$2\times12d;2\times12e$ $2\times24f$	$2\times24f$ $4\times24f$
[4] $I23$ (197)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$8c$	$2a;6b$	$12d;12e$	$24f$	$8c;24f$ $2\times24f$	$2\times24f$ $2\times12d;2\times12e$	$2\times24f$ $4\times24f$

	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$3c$ $6g$	$3d$ $6h$	$4e$ $6i$	$6f$ $12j$
Enlarged unit cell, isomorphic								
[27] $P23$	$3\mathbf{a},3\mathbf{b},3\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z;\pm(\frac{1}{3},0,0);$ $\pm(0,\frac{1}{3},0);\pm(0,0,\frac{1}{3});$ $\pm(0,\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},0,\frac{1}{3});$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(0,\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},0,\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$1a;2\times4e;6f;$ $12j$	$1b;2\times4e;6i;$ $12j$	$3c;6g;6h;$ $6i;5\times12j$ $3\times6g;$ $12\times12j$	$3d;6f;6g;$ $6h;5\times12j$ $3\times6h;$ $12\times12j$	$3\times4e;$ $8\times12j$ $3\times12i;$ $12\times12j$	$3\times6f;$ $12\times12j$ $27\times12j$
[p^3] $P23$	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$ $p=$ prime $>2;$	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z;$ $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w=1,\ldots,p-1$	$1a;(p-1)\times4e;$ $\frac{p-1}{2}\times6f;$ $\frac{(p-1)(p-2)(p+3)}{12}\times12j$	$1b;(p-1)\times4e;$ $\frac{p-1}{2}\times6i;$ $\frac{(p-1)(p-2)(p+3)}{12}\times12j$	$3c;\frac{p-1}{2}\times6g;$ $\frac{p-1}{2}\times6h;$ $\frac{p-1}{2}\times6i;$ $\frac{(p-1)^2(p+2)}{4}\times$ $12j$ $p\times6g;$ $\frac{p(p^2-1)}{2}\times12j$	$3d;\frac{p-1}{2}\times6f;$ $\frac{p-1}{2}\times6g;$ $\frac{p-1}{2}\times6h;$ $\frac{(p-1)^2(p+2)}{4}\times$ $12j$ $p\times6h;$ $\frac{p(p^2-1)}{2}\times12j$	$p\times4e;$ $\frac{p(p^2-1)}{3}\times12j$ $p\times6i;$ $\frac{p(p^2-1)}{2}\times12j$	$p\times6f;$ $\frac{p(p^2-1)}{2}\times12j$ $p^3\times12j$

$F23$ No. 196 T^2

	Axes	Coordinates	Wyckoff positions 4*a*	4*b*	4*c*	4*d*	16*e* 24*g*	24*f* 48*h*
I Maximal *translationengleiche* subgroups								
[4] $R3$ (146)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhombo. axes)	$-x+y+z$, $x-y+z$, $x+y-z$	1*a*	1*a*	1*a*	1*a*	1*a*; 3*b* 2×3*b*	2×3*b* 4×3*b*
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}+\mathbf{c})$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z)$, $\frac{2}{3}(-x-y+2z)$, $\frac{1}{3}(x+y+z)$	3*a*	3*a*	3*a*	3*a*	3*a*; 9*b* 2×9*b*	2×9*b* 4×9*b*
conjugate:	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}-\mathbf{c})$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z)$, $\frac{2}{3}(x-y-2z)$, $\frac{1}{3}(-x+y-z)$						
conjugate:	$\frac{1}{2}(-\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}-\mathbf{c})$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z)$, $\frac{2}{3}(-x+y-2z)$, $\frac{1}{3}(x-y-z)$						
conjugate:	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}+\mathbf{c})$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z)$, $\frac{2}{3}(x+y+2z)$, $\frac{1}{3}(-x-y+z)$						
[3] $F222$ (22)			4*a*	4*b*	4*c*	4*d*	16*k* 8*h*; 8*i*; 8*j*	8*e*; 8*f*; 8*g* 3×16*k*
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[4] $P2_13$ (198) 4 conjugate subgroups			4*a*	4*a*	4*a*	4*a*	4*a*; 12*b* 2×12*b*	2×12*b* 4×12*b*
[4] $P2_13$ (198) 4 conjugate subgroups		$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	4*a*	4*a*	4*a*	4*a*	4*a*; 12*b* 2×12*b*	2×12*b* 4×12*b*
[4] $P23$ (195) 4 conjugate subgroups			1*a*; 3*c*	1*b*; 3*d*	4*e*	4*e*	4*e*; 12*j* 2×12*j*	6*f*; 6*g*; 6*h*; 6*i* 4×12*j*
[4] $P23$ (195) 4 conjugate subgroups		$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	4*e*	4*e*	1*b*; 3*d*	1*a*; 3*c*	4*e*; 12*j* 6*f*; 6*g*; 6*h*; 6*i*	2×12*j* 4×12*j*
Enlarged unit cell, isomorphic								
[27] $F23$	3**a**, 3**b**, 3**c**	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	4*a*; 2×16*e*; 24*f*; 48*h*	4*b*; 2×16*e*; 24*f*; 48*h*	4*d*; 2×16*e*; 24*g*; 48*h*	4*c*; 2×16*e*; 24*g*; 48*h*	3×16*e*; 8×48*h* 3×24*g*; 12×48*h*	3×24*f*; 12×48*h* 27×48*h*
$[p^3]$ $F23$	p**a**, p**b**, p**c** p = prime > 2; $u,v,w = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	4*a*; $(p-1)\times16e$; $\frac{p-1}{2}\times24f$; $\frac{p^3-7p+6}{12}\times48h$	4*b*; $(p-1)\times16e$; $\frac{p-1}{2}\times24f$; $\frac{p^3-7p+6}{12}\times48h$	$4c(d^*)$; $(p-1)\times16e$; $\frac{p-1}{2}\times24g$; $\frac{p^3-7p+6}{12}\times48h$	$4d(c^*)$; $(p-1)\times16e$; $\frac{p-1}{2}\times24g$; $\frac{p^3-7p+6}{12}\times48h$	$p\times16e$; $\frac{p(p^2-1)}{3}\times48h$ $p\times24g$; $\frac{p(p^2-1)}{2}\times48h$	$p\times24f$; $\frac{p(p^2-1)}{2}\times48h$ $p^3\times48h$

* $p = 4n-1$

T^3 No. 197 $I23$

	Axes	Coordinates	Wyckoff positions					
			$2a$	$6b$	$8c$	$12d$	$12e$	$24f$
I Maximal *translationengleiche* subgroups								
[4] $R3$ (146)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	$1a$	$3b$	$1a; 3b$	$2\times 3b$	$2\times 3b$	$4\times 3b$
	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z), \frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)$	$3a$	$9b$	$3a; 9b$	$2\times 9b$	$2\times 9b$	$4\times 9b$
	conjugate: $\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z), \frac{1}{3}(x-y-2z)$, $\frac{2}{3}(-x+y-z)$						
	conjugate: $-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z), \frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$						
	conjugate: $\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z), \frac{1}{3}(x+y+2z)$, $\frac{2}{3}(-x-y+z)$						
[3] $I222$ (23)			$2a$	$2b; 2c; 2d$	$8k$	$4e; 4g; 4i$	$4f; 4h; 4j$	$3\times 8k$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P23$ (195)			$1a; 1b$	$3c; 3d$	$2\times 4e$	$6f; 6i$	$6g; 6h$	$2\times 12j$
Enlarged unit cell, isomorphic								
[27] $I23$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$2a; 2\times 8c; 12d; 24f$	$6b; 12d; 2\times 12e; 5\times 24f$	$3\times 8c; 8\times 24f$	$3\times 12d; 12\times 24f$	$3\times 12e; 12\times 24f$	$27\times 24f$
$[p^3]$ $I23$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime > 2; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$2a; (p-1)\times 8c$; $\frac{p-1}{2}\times 12d$; $\frac{(p-1)(p-2)(p+3)}{12}\times 24f$	$6b; \frac{p-1}{2}\times 12d$; $(p-1)\times 12e$; $\frac{(p-1)^2(p+2)}{4}\times 24f$	$p\times 8c$; $\frac{p(p^2-1)}{3}\times 24f$	$p\times 12d$; $\frac{p(p^2-1)}{2}\times 24f$	$p\times 12e$; $\frac{p(p^2-1)}{2}\times 24f$	$p^3\times 24f$

$P2_13$ No. 198 T^4

	Axes	Coordinates	Wyckoff positions 4a	12b
I Maximal *translationengleiche* subgroups				
[4] $R3$ (146)	(rhombohedral axes)		$1a; 3b$	$4\times 3b$
	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y-z), \frac{1}{3}(x+y-2z), \frac{1}{3}(x+y+z)$	$3a; 9b$	$4\times 9b$
	conjugate: $-\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}, -\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z), \frac{1}{3}(-x+y+2z)-\frac{1}{2}, \frac{1}{3}(-x+y-z)$		
	conjugate: $\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}, \mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z)-\frac{1}{2}, \frac{1}{3}(x-y+2z), \frac{1}{3}(x-y-z)$		
	conjugate: $-\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}, -\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}, \frac{1}{3}(-x-y-2z)+\frac{1}{2}, \frac{1}{3}(-x-y+z)$		
[3] $P2_12_12_1$ (19)			$4a$	$3\times 4a$
II Maximal *klassengleiche* subgroups				
Enlarged unit cell, isomorphic				
[27] $P2_13$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{1}{3}); \pm(0,\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0); \pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$3\times 4a; 8\times 12b$	$27\times 12b$
$[p^3]$ $P2_13$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$; $u,v,w = 1,\ldots,p-1$	$p\times 4a; \frac{p(p^2-1)}{3}\times 12b$	$p^3\times 12b$

T^5 No. 199 $I2_13$

Axes		Coordinates	8*a*	12*b*	24*c*
I Maximal *translationengleiche* subgroups					
[4] $R3$ (146)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	$1a; 3b$	$2\times3b$	$4\times3b$
	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z)$, $\frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)$	$3a; 9b$	$2\times9b$	$4\times9b$
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z)$, $\frac{1}{3}(x-y-2z)+\frac{1}{2}$, $\frac{2}{3}(-x+y-z)$			
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$			
	conjugate: $\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z)-\frac{1}{2}$, $\frac{1}{3}(x+y+2z)-\frac{1}{2}$, $\frac{2}{3}(-x-y+z)$			
[3] $I2_12_12_1$ (24)			$8d$	$4a; 4b; 4c$	$3\times8d$
II Maximal *klassengleiche* subgroups					
Loss of centring translations					
[2] $P2_13$ (198)			$2\times4a$	$12b$	$2\times12b$
Enlarged unit cell, isomorphic					
[27] $I2_13$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$3\times8a; 8\times24c$	$3\times12b; 12\times24c$	$27\times24c$
$[p^3]$ $I2_13$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$; $u,v,w = 1,\ldots,p-1$	$p\times8a; \frac{p(p^2-1)}{3}\times24c$	$p\times12b; \frac{p(p^2-1)}{2}\times24c$	$p^3\times24c$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 200, pp. 684–685.

$Pm\bar{3}$ No. 200 $P2/m\bar{3}$ T_h^1

	Axes	Coordinates	Wyckoff positions						
			$1a$	$1b$	$3c$ $6h$	$3d$ $8i$	$6e$ $12j$	$6f$ $12k$	$6g$ $24l$
I Maximal *translationengleiche* subgroups									
[2] $P23$ (195)			$1a$	$1b$	$3c$ $6i$	$3d$ $2\times4e$	$6f$ $12j$	$6g$ $12j$	$6h$ $2\times12j$
[4] $R\bar{3}$ (148)	(rhombohedral axes)		$1a$	$1b$	$3e$ $6f$	$3d$ $2c;6f$	$6f$ $2\times6f$	$6f$ $2\times6f$	$6f$ $4\times6f$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$3a$	$3b$	$9e$ $18f$	$9d$ $6c;18f$	$18f$ $2\times18f$	$18f$ $2\times18f$	$18f$ $4\times18f$
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)$							
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)$							
	conjugate: $-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z)$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$							
[3] $Pmmm$ (47)			$1a$	$1h$	$1d;1f;1g$ $2l;2p;2t$	$1b;1c;1e$ 8α	$2i;2m;2q$ $4u;4w;4y$	$2j;2o;2r$ $4v;4x;4z$	$2k;2n;2s$ $3\times8\alpha$
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**									
[2] $Fm\bar{3}$ (202)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$4a;4b$	$8c$	$24d$ $48g$	$24e$ $2\times32f$	$2\times24e$ $2\times48h$	$48h$ $96i$	$48h$ $2\times96i$
[2] $Fm\bar{3}$ (202)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$8c$	$4a;4b$	$24e$ $2\times24e$	$24d$ $2\times32f$	$48g$ $96i$	$48h$ $2\times48h$	$48h$ $2\times96i$
[4] $Ia\bar{3}$ (206)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$8a$	$8b$	$24d$ $48e$	$24d$ $16c;48e$	$48e$ $2\times48e$	$2\times24d$ $2\times48e$	$48e$ $4\times48e$
[4] $Ia\bar{3}$ (206)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$8b$	$8a$	$24d$ $48e$	$24d$ $16c;48e$	$48e$ $2\times48e$	$48e$ $2\times48e$	$2\times24d$ $4\times48e$
[4] $Im\bar{3}$ (204)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$2a;6b$	$8c$	$24g$ $48h$	$12d;12e$ $16f;48h$	$2\times12d;2\times12e$ $4\times24g$	$2\times24g$ $2\times48h$	$2\times24g$ $4\times48h$
[4] $Im\bar{3}$ (204)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$8c$	$2a;6b$	$12d;12e$ $2\times12d;2\times12e$	$24g$ $16f;48h$	$48h$ $2\times48h$	$2\times24g$ $4\times24g$	$2\times24g$ $4\times48h$

	Axes	Coordinates	Wyckoff positions 1a / 6g	1b / 6h	3c / 8i	3d / 12j	6e / 12k	6f / 24l
Enlarged unit cell, isomorphic								
[27] $Pm\bar{3}$	3**a**,3**b**,3**c**	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z;\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);\pm(0,0,\frac{1}{3});\pm(0,\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},0,\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},0);\pm(0,\frac{1}{3},\frac{2}{3});\pm(\frac{1}{3},0,\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},0);\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$1a;6e;8i;12j$	$1b;6h;8i;12k$	$3c;6f;6g;6h;12j;2\times12k;24l$	$3d;6e;6f;6g;2\times12j;12k;24l$	$3\times6e;6\times12j;3\times24l$	$3\times6f;3\times12j;3\times12k;3\times24l$
			$3\times6g;3\times12j;3\times12k;3\times24l$	$3\times6h;6\times12k;3\times24l$	$3\times8i;8\times24l$	$9\times12j;9\times24l$	$9\times12k;9\times24l$	$27\times24l$
[p^3] $Pm\bar{3}$	p**a**,p**b**,p**c** p = prime >2;	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z;+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w=1,\dots,p-1$	$1a;\frac{p-1}{2}\times6e;\frac{p-1}{2}\times8i;\frac{(p-1)^2}{4}\times12j;\frac{(p^2-1)(p-3)}{24}\times24l$	$1b;\frac{p-1}{2}\times6h;\frac{p-1}{2}\times8i;\frac{(p-1)^2}{4}\times12k;\frac{(p^2-1)(p-3)}{24}\times24l$	$3c;\frac{p-1}{2}\times6f;\frac{p-1}{2}\times6g;\frac{p-1}{2}\times6h;\frac{(p-1)^2}{4}\times12j;\frac{(p-1)^2}{2}\times12k;\frac{(p-1)^3}{8}\times24l$	$3d;\frac{p-1}{2}\times6e;\frac{p-1}{2}\times6f;\frac{p-1}{2}\times6g;\frac{(p-1)^2}{2}\times12j;\frac{(p-1)^2}{4}\times12k;\frac{(p-1)^3}{8}\times24l$	$p\times6e;p(p-1)\times12j;\frac{p(p-1)^2}{4}\times24l$	$p\times6f;\frac{p(p-1)}{2}\times12j;\frac{p(p-1)}{2}\times12k;\frac{p(p-1)^2}{4}\times24l$
			$p\times6g;\frac{p(p-1)}{2}\times12j;\frac{p(p-1)}{2}\times12k;\frac{p(p-1)^2}{4}\times24l$	$p\times6h;p(p-1)\times12k;\frac{p(p-1)^2}{4}\times24l$	$p\times8i;\frac{p(p^2-1)}{3}\times24l$	$p^2\times12j$ $\frac{p^2(p-1)}{2}\times24l$	$p^2\times12k$ $\frac{p^2(p-1)}{2}\times24l$	$p^3\times24l$

$Pn\bar{3}$ No. 201 $P2/n\bar{3}$ T_h^2

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions $2a$	$4b$	$4c$	$6d$	$8e$ $12g$	$12f$ $24h$
I Maximal *translationengleiche* subgroups									
[2] $P23$ (195)			$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$1a;1b$	$4e$	$4e$	$3c;3d$	$2\times4e$ $6g;6h$	$6f;6i$ $2\times12j$
[4] $R\bar{3}$ (148) (rhombohedral axes)		$x-\frac{1}{4},y-\frac{1}{4},z-\frac{1}{4}$		$2c$	$1a;3e$	$1b;3d$	$6f$	$2c;6f$ $2\times6f$	$2\times6f$ $4\times6f$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)-\frac{1}{4}$	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$6c$	$3a;9e$	$3b;9d$	$18f$	$6c;18f$ $2\times18f$	$2\times18f$ $4\times18f$
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)-\frac{1}{4}$	$\frac{1}{3}(-2x-y+z)+\frac{1}{2}$, $\frac{1}{3}(-x+y+2z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-z)$						
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)-\frac{1}{4}$	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)+\frac{1}{2}$, $\frac{1}{3}(x-y-z)$						
	conjugate: $-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x+y-z)$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)-\frac{1}{4}$	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$						
[3] $Pnnn$ (48)				$2a$	$4e(f^*)$	$4f(e^*)$	$2b;2c;2d$	$8m$ $4h;4j;4l$	$4g;4i;4k$ $3\times8m$

* origin 2

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$4b$	$4c$	$6d$	$8e$ $12g$	$12f$ $24h$
[2] $Fd\bar{3}$ (203)	$2\mathbf{a}$, $2\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$8a;8b$	$16c;16d$	$32e$	$48f$	$2\times32e$ $96g$	$2\times48f$ $2\times96g$
[2] $Fd\bar{3}$ (203)	$2\mathbf{a}$, $2\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4}$, $\frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4}$, $\frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$8a;8b$	$32e$	$16c;16d$	$48f$	$2\times32e$ $96g$	$2\times48f$ $2\times96g$

Enlarged unit cell, isomorphic

	Axes	Coordinates origin 1	Coordinates origin 2	$2a$	$4b$	$4c$	$6d$	$8e$ $12g$	$12f$ $24h$
[27] $Pn\bar{3}$	$3\mathbf{a}$, $3\mathbf{b}$, $3\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z$;	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z$;	$2a;2\times8e$; $12f;24h$	$4b(c^\dagger);8e$; $4\times24h$	$4c(b^\dagger);8e$; $4\times24h$	$6d;12f$; $2\times12g$; $5\times24h$	$3\times8e$; $8\times24h$ $3\times12g$; $12\times24h$	$3\times12f$; $12\times24h$ $27\times24h$
		$\underbrace{\qquad\qquad\qquad}$ $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$							
$[p^3]$ $Pn\bar{3}$	$p\mathbf{a}$, $p\mathbf{b}$, $p\mathbf{c}$ $p=\text{prime}>2$; $u,v,w=1,\ldots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$2a$; $(p-1)\times8e$; $\frac{p-1}{2}\times12f$; $\frac{p^3-7p+6}{12}\times24h$	$4b(c^\ddagger)$; $\frac{p-1}{2}\times8e$; $\frac{p(p^2-1)}{6}\times24h$	$4c(b^\ddagger)$; $\frac{p-1}{2}\times8e$; $\frac{p(p^2-1)}{6}\times24h$	$6d;\frac{p-1}{2}\times12f$ $(p-1)\times12g$; $\frac{(p-1)^2(p+2)}{4}\times24h$	$p\times8e$; $\frac{p(p^2-1)}{3}\times24h$ $p\times12g$; $\frac{p(p^2-1)}{2}\times24h$	$p\times12f$; $\frac{p(p^2-1)}{2}\times24h$ $p^3\times24h$

† origin 1

‡ origin 1 and $p=4n-1$

T_h^3 $F\,2/m\,\bar{3}$ No. 202 $F\,m\,\bar{3}$

	Axes	Coordinates	$4a$	$4b$	$8c$	$24d$ $48g$	$24e$ $48h$	$32f$ $96i$
I Maximal *translationengleiche* subgroups								
[2] $F23$ (196)			$4a$	$4b$	$4c; 4d$	$24g$ $2\times 24g$	$24f$ $48h$	$2\times 16e$ $2\times 48h$
[4] $R\bar{3}$ (148)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhomboh. axes)	$-x+y+z$, $x-y+z$, $x+y-z$	$1a$	$1b$	$2c$	$3d; 3e$ $2\times 6f$	$6f$ $2\times 6f$	$2c; 6f$ $4\times 6f$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}+\mathbf{c}), \mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z)$, $\frac{2}{3}(-x-y+2z)$, $\frac{1}{3}(x+y+z)$	$3a$	$3b$	$6c$	$9d; 9e$ $2\times 18f$	$18f$ $2\times 18f$	$6c; 18f$ $4\times 18f$
	conjugate: $\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}-\mathbf{c}), -\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z)$, $\frac{2}{3}(x-y-2z)$, $\frac{1}{3}(-x+y-z)$						
	conjugate: $\frac{1}{2}(-\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}-\mathbf{c}), \mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z)$, $\frac{2}{3}(-x+y-2z)$, $\frac{1}{3}(x-y-z)$						
	conjugate: $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}+\mathbf{c}), -\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z)$, $\frac{2}{3}(x+y+2z)$, $\frac{1}{3}(-x-y+z)$						
[3] $Fmmm$ (69)			$4a$	$4b$	$8f$	$8c; 8d; 8e$ $16j; 16k; 16l$	$8g; 8h; 8i$ $16m; 16n; 16o$	$32p$ $3\times 32i$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[4] $Pa\bar{3}$ (205) 4 conjugate subgroups			$4a$	$4b$	$8c$	$24d$ $2\times 24d$	$24d$ $2\times 24d$	$8c; 24d$ $4\times 24d$
[4] $Pa\bar{3}$ (205)	$-\mathbf{b}, \mathbf{a}, \mathbf{c}$ 4 conjugate subgroups	$-y, x, z$	$4a$	$4b$	$8c$	$24d$ $2\times 24d$	$24d$ $2\times 24d$	$8c; 24d$ $4\times 24d$
[4] $Pn\bar{3}$ (201) 4 conju. subgr.		origin 1: $x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$ origin 2: x, y, z	$4b$	$4c$	$2a; 6d$	$12f; 12g$ $2\times 12f; 2\times 12g$	$24h$ $2\times 24h$	$8e; 24h$ $4\times 24h$
[4] $Pm\bar{3}$ (200) 4 conjugate subgroups			$1a; 3c$	$1b; 3d$	$8i$	$12j; 12k$ $2\times 24l$	$6e; 6f; 6g; 6h$ $2\times 12j; 2\times 12k$	$8i; 24l$ $4\times 24l$
Enlarged unit cell, isomorphic								
[27] $Fm\bar{3}$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$4a; 24e; 32f;$ $48h$	$4b; 24e; 32f;$ $48h$	$8c; 2\times 32f;$ $48g; 96i$	$24d; 48g;$ $4\times 48h;$ $4\times 96i$ $3\times 48g;$ $12\times 96i$	$3\times 24e;$ $6\times 48h;$ $3\times 96i$ $9\times 48h; 9\times 96i$	$3\times 32f;$ $8\times 96i$ $27\times 96i$
$[p^3]$ $Fm\bar{3}$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime >2; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$4a; \frac{p-1}{2}\times 24e;$ $\frac{p-1}{2}\times 32f;$ $\frac{(p-1)^2}{4}\times 48h;$ $\frac{(p^2-1)(p-3)}{24}\times 96i$	$4b; \frac{p-1}{2}\times 24e;$ $\frac{p-1}{2}\times 32f;$ $\frac{(p-1)^2}{4}\times 48h;$ $\frac{(p^2-1)(p-3)}{24}\times 96i$	$8c;$ $(p-1)\times 32f;$ $\frac{p-1}{2}\times 48g;$ $\frac{p^3-7p+6}{12}\times 96i$	$24d;$ $\frac{p-1}{2}\times 48g;$ $\frac{p^2-1}{2}\times 48h;$ $\frac{(p^2-1)(p-1)}{4}\times 96i$ $p\times 48g;$ $\frac{p(p^2-1)}{2}\times 96i$	$p\times 24e;$ $p(p-1)\times 48h;$ $\frac{p(p-1)^2}{4}\times 96i$ $p^2\times 48h$ $\frac{p^2(p-1)}{2}\times 96i$	$p\times 32f;$ $\frac{p(p^2-1)}{3}\times 96i$ $p^3\times 96i$

$Fd\bar{3}$ No. 203 $F\,2/d\,\bar{3}$ T_h^4

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions 8a	8b	16c	16d	32e	48f 96g
I Maximal *translationengleiche* subgroups									
[2] $F23$ (196)			$x+\frac{1}{8}, y+\frac{1}{8}, z+\frac{1}{8}$	4a; 4c	4b; 4d	16e	16e	2×16e	24f; 24g 2×48h
[4] $R\bar{3}$ (148)	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhombohedral axes)	$-x+y+z-\frac{1}{8}$, $x-y+z-\frac{1}{8}$, $x+y-z-\frac{1}{8}$	$-x+y+z$, $x-y+z$, $x+y-z$	2c	2c	1a; 3d	1b; 3e	2c; 6f	2×6f 4×6f
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(-\mathbf{b}+\mathbf{c})$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z)$, $\frac{2}{3}(-x-y+2z)$, $\frac{1}{3}(x+y+z)-\frac{1}{8}$	$\frac{2}{3}(-2x+y+z)$, $\frac{2}{3}(-x-y+2z)$, $\frac{1}{3}(x+y+z)$	6c	6c	3a; 9d	3b; 9e	6c; 18f	2×18f 4×18f
conjugate:	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(-\mathbf{b}-\mathbf{c})$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z)$, $\frac{2}{3}(x-y-2z)$, $\frac{1}{3}(-x+y-z)-\frac{1}{8}$	$\frac{2}{3}(2x+y-z)+\frac{1}{2}$, $\frac{2}{3}(x-y-2z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-z)+\frac{1}{2}$						
conjugate:	$\frac{1}{2}(-\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{b}-\mathbf{c})$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z)$, $\frac{2}{3}(-x+y-2z)$, $\frac{1}{3}(x-y-z)-\frac{1}{8}$	$\frac{2}{3}(-2x-y-z)$, $\frac{2}{3}(-x+y-2z)+\frac{1}{2}$, $\frac{1}{3}(x-y-z)+\frac{1}{2}$						
conjugate:	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z)$, $\frac{2}{3}(x+y+2z)$, $\frac{1}{3}(-x-y+z)-\frac{1}{8}$	$\frac{2}{3}(2x-y+z)+\frac{1}{2}$, $\frac{2}{3}(x+y+2z)$, $\frac{1}{3}(-x-y+z)+\frac{1}{2}$						
[3] $Fddd$ (70)				8a	8b	16c	16d	32h	16e; 16f; 16g 3×32h
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**									
[27] $Fd\bar{3}$	3**a**, 3**b**, 3**c**	$\frac{1}{3}x-\frac{1}{4}, \frac{1}{3}y-\frac{1}{4}, \frac{1}{3}z-\frac{1}{4}$;	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$;	8b; 2×32e; 48f; 96g	8a; 2×32e; 48f; 96g	16c; 32e; 4×96g	16d; 32e; 4×96g	3×32e; 8×96g	3×48f; 12×96g 27×96g
		$\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$							
[p^3] $Fd\bar{3}$	p**a**, p**b**, p**c**	$\frac{1}{p}x+s, \frac{1}{p}y+s, \frac{1}{p}z+s$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	8a(b^*); $(p-1)$×32e; $\frac{p-1}{2}$×48f; $\frac{p^3-7p+6}{12}$×96g	4b(a^*); $(p-1)$×32e; $\frac{p-1}{2}$×48f; $\frac{p^3-7p+6}{12}$×96g	16c; $\frac{p-1}{2}$×32e; $\frac{p(p^2-1)}{6}$×96g	16d; $\frac{p-1}{2}$×32e; $\frac{p(p^2-1)}{6}$×96g	p×32e; $\frac{p(p^2-1)}{3}$×96g	p×48f; $\frac{p(p^2-1)}{2}$×96g p^3×96g
	p = prime > 2; $u,v,w = 1,\ldots,p-1$; $s = 0$ if $p = 8n+1$; $s = -\frac{1}{4}$ if $p = 8n+3$; $s = \frac{1}{2}$ if $p = 8n+5$; $s = \frac{1}{4}$ if $p = 8n+7$								

$^*\,p = 8n\pm 3$

T_h^5 $I2/m\bar{3}$ No. 204 $Im\bar{3}$

	Axes	Coordinates	Wyckoff positions $2a$	 $6b$	 $8c$	 $12d$	 $12e$ $24g$	 $16f$ $48h$
I Maximal *translationengleiche* subgroups								
[2] $I23$ (197)			$2a$	$6b$	$8c$	$12d$	$12e$ $24f$	$2\times8c$ $2\times24f$
[4] $R\bar{3}$ (148)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	$1a$	$3e$	$1b; 3d$	$6f$	$6f$ $2\times6f$	$2c; 6f$ $4\times6f$
	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z)$, $\frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)$	$3a$	$9e$	$3b; 9d$	$18f$	$18f$ $2\times18f$	$6c; 18f$ $4\times18f$
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z)$, $\frac{1}{3}(x-y-2z)$, $\frac{2}{3}(-x+y-z)$						
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z)$, $\frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$						
	conjugate: $\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z)$, $\frac{1}{3}(x+y+2z)$, $\frac{2}{3}(-x-y+z)$						
[3] $Immm$ (71)			$2a$	$2b; 2c; 2d$	$8k$	$4e; 4g; 4i$	$4f; 4h; 4j$ $8l; 8m; 8n$	$16o$ $3\times16o$
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $Pn\bar{3}$ (201)		origin 1: x, y, z origin 2: $x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$2a$	$6d$	$4b; 4c$	$12f$	$12g$ $24h$	$2\times8e$ $2\times24h$
[2] $Pm\bar{3}$ (200)			$1a; 1b$	$3c; 3d$	$8i$	$6e; 6h$	$6f; 6g$ $12j; 12k$	$2\times8i$ $2\times24l$
Enlarged unit cell, isomorphic								
[27] $Im\bar{3}$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$2a$; $12d$; $16f$; $24g$	$6b$; $12d$; $2\times12e$; $3\times24g$; $48h$	$8c$; $16f$; $4\times48h$	$3\times12d$; $6\times24g$; $3\times48h$	$3\times12e$; $6\times24g$; $3\times48h$ $9\times24g$; $9\times48h$	$3\times16f$; $8\times48h$ $27\times48h$
$[p^3]$ $Im\bar{3}$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$2a$; $\frac{p-1}{2}\times12d$; $\frac{p-1}{2}\times16f$; $\frac{(p-1)^2}{4}\times24g$; $\frac{(p^2-1)(p-3)}{24}\times48h$	$6b$; $\frac{p-1}{2}\times12d$; $(p-1)\times12e$; $\frac{3(p-1)^2}{4}\times24g$; $\frac{(p-1)^3}{8}\times48h$	$8c$; $\frac{p-1}{2}\times16f$; $\frac{p(p^2-1)}{6}\times48h$	$p\times12d$; $p(p-1)\times24g$; $\frac{p(p-1)^2}{4}\times48h$	$p\times12e$; $p(p-1)\times24g$; $\frac{p(p-1)^2}{4}\times48h$ $p^2\times24g$; $\frac{p^2(p-1)}{2}\times48h$	$p\times16f$; $\frac{p(p^2-1)}{3}\times48h$ $p^3\times48h$

$Pa\bar{3}$ No. 205 $P2_1/a\bar{3}$ T_h^6

	Axes	Coordinates	$4a$	$4b$	$8c$	$24d$
I Maximal *translationengleiche* subgroups						
[2] $P2_13$ (198)			$4a$	$4a$	$2\times4a$	$2\times12b$
[4] $R\bar{3}$ (148)	(rhombohedral axes)		$1a; 3e$	$1b; 3d$	$2c; 6f$	$4\times6f$
	a−**b**, **b**−**c**, **a**+**b**+**c** (hexagonal axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$3a; 9e$	$3b; 9d$	$6c; 18f$	$4\times18f$
	conjugate: −**a**−**b**, **b**+**c**, −**a**+**b**−**c** (hexagonal axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)-\frac{1}{2}$, $\frac{1}{3}(-x+y-z)$				
	conjugate: **a**+**b**, −**b**+**c**, **a**−**b**−**c** (hexagonal axes)	$\frac{1}{3}(2x+y+z)-\frac{1}{2}$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)$				
	conjugate: −**a**+**b**, −**b**−**c**, −**a**−**b**+**c** (hexagonal axes)	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}$, $\frac{1}{3}(-x-y-2z)+\frac{1}{2}$, $\frac{1}{3}(-x-y+z)$				
[3] $Pbca$ (61)			$4a$	$4b$	$8c$	$3\times8c$
II Maximal *klassengleiche* subgroups						
Enlarged unit cell, isomorphic						
[27] $Pa\bar{3}$	3**a**, 3**b**, 3**c**	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$4a; 8c; 4\times24d$	$4b; 8c; 4\times24d$	$3\times8c; 8\times24d$	$27\times24d$
$[p^3]$ $Pa\bar{3}$	p**a**, p**b**, p**c**; p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$; $u,v,w = 1,\ldots,p-1$	$4a; \frac{p-1}{2}\times8c$; $\frac{p(p^2-1)}{6}\times24d$	$4b; \frac{p-1}{2}\times8c$; $\frac{p(p^2-1)}{6}\times24d$	$p\times8c$; $\frac{p(p^2-1)}{3}\times24d$	$p^3\times24d$

T_h^7 $I2_1/a\bar{3}$ No. 206 $Ia\bar{3}$

I Maximal *translationengleiche* subgroups

Subgroup	Axes	Coordinates	8*a*	8*b*	16*c*	24*d*	48*e*
[2] $I2_13$ (199)			8*a*	8*a*	2×8*a*	2×12*b*	2×24*c*
[4] $R\bar{3}$ (148)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	1*a*; 3*e*	1*b*; 3*d*	2*c*; 6*f*	2×6*f*	4×6*f*
	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z)$, $\frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)$	3*a*; 9*e*	3*b*; 9*d*	6*c*; 18*f*	2×18*f*	4×18*f*
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z)$, $\frac{1}{3}(x-y-2z)+\frac{1}{2}$, $\frac{2}{3}(-x+y-z)$					
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$					
	conjugate: $\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z)-\frac{1}{2}$, $\frac{1}{3}(x+y+2z)-\frac{1}{2}$, $\frac{2}{3}(-x-y+z)$					
[3] *Ibca* (73)			8*a*	8*b*	16*f*	8*c*; 8*d*; 8*e*	3×16*f*

II Maximal *klassengleiche* subgroups

Loss of centring translations

Subgroup	Axes	Coordinates	8*a*	8*b*	16*c*	24*d*	48*e*
[2] $Pa\bar{3}$ (205)			4*a*; 4*b*	8*c*	2×8*c*	24*d*	2×24*d*
[2] $Pa\bar{3}$ (205)	$-\mathbf{b}$, $\mathbf{a}$, $\mathbf{c}$	$-y+\frac{1}{4}, x-\frac{1}{4}, z+\frac{1}{4}$	8*c*	4*a*; 4*b*	2×8*c*	24*d*	2×24*d*

Enlarged unit cell, isomorphic

Subgroup	Axes	Coordinates	8*a*	8*b*	16*c*	24*d*	48*e*
[27] $Ia\bar{3}$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	8*a*; 16*c*; 4×48*e*	8*b*; 16*c*; 4×48*e*	3×16*c*; 8×48*e*	3×24*d*; 12×48*e*	27×48*e*
$[p^3]$ $Ia\bar{3}$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$; $u,v,w = 1,\ldots,p-1$	8*a*; $\frac{p-1}{2}\times$16*c*; $\frac{p(p^2-1)}{6}\times$48*e*	8*b*; $\frac{p-1}{2}\times$16*c*; $\frac{p(p^2-1)}{6}\times$48*e*	$p\times$16*c*; $\frac{p(p^2-1)}{3}\times$48*e*	$p\times$24*d*; $\frac{p(p^2-1)}{2}\times$48*e*	$p^3\times$48*e*

$P432$ No. 207 O^1

	Axes	Coordinates	Wyckoff positions $1a$	 $1b$ $8g$	 $3c$ $12h$	 $3d$ $12i$	 $4e$ $12j$	 $6f$ $24k$
I Maximal *translationengleiche* subgroups								
[2] $P23$ (195)			$1a$	$1b$ $2\times4e$	$3c$ $6g;6h$	$3d$ $12j$	$6f$ $12j$	$6i$ $2\times12j$
[4] $R32$ (155)	(rhombohedral axes)		$1a$	$1b$ $2c;6f$	$3d$ $2\times6f$	$3e$ $2\times3d;6f$	$6f$ $2\times3e;6f$	$6f$ $4\times6f$
(hex. axes)	$\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \mathbf{a}+\mathbf{b}+\mathbf{c}$	$\frac{1}{3}(2x-y-z), \frac{1}{3}(x+y-2z), \frac{1}{3}(x+y+z)$	$3a$	$3b$ $6c;18f$	$9d$ $2\times18f$	$9e$ $2\times9d;18f$	$18f$ $2\times9e;18f$	$18f$ $4\times18f$
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}, -\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z), \frac{1}{3}(-x+y+2z), \frac{1}{3}(-x+y-z)$						
conjugate:	$\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}, \mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z), \frac{1}{3}(x-y+2z), \frac{1}{3}(x-y-z)$						
conjugate:	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}, -\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z), \frac{1}{3}(-x-y-2z), \frac{1}{3}(-x-y+z)$						
[3] $P422$ (89) conjugate: conjugate:	 $\mathbf{b},\mathbf{c},\mathbf{a}$ $\mathbf{c},\mathbf{a},\mathbf{b}$	 y,z,x z,x,y	$1a$	$1d$ $8p$	$1c;2f$ $4i;4n;4o$	$1b;2e$ $4j;8p$	$2g;4l$ $4k;8p$	$2h;4m$ $3\times8p$
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[2] $F432$ (209)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z; +(\frac{1}{2},0,0)$	$4a;4b$	$8c$ $2\times32f$	$24d$ $96j$	$24e$ $48g;48h$	$2\times24e$ $96j$	$48i$ $2\times96j$
[2] $F432$ (209)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2},0,0)$	$8c$	$4a;4b$ $2\times32f$	$24e$ $96j$	$24d$ $96j$	$48i$ $48g;48h$	$2\times24e$ $2\times96j$
[4] $I432$ (211)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(0,0,\frac{1}{2})$	$2a;6b$	$8c$ $16f;48j$	$24h$ $2\times48j$	$12d;12e$ $2\times24h;48j$	$2\times12e;24g$ $2\times24i;48j$	$48j$ $4\times48j$
[4] $I432$ (211)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(0,0,\frac{1}{2})$	$8c$	$2a;6b$ $16f;48j$	$12d;12e$ $2\times48j$	$24h$ $2\times24i;48j$	$48j$ $2\times24h;48j$	$2\times12e;24g$ $4\times48j$
Enlarged unit cell, isomorphic								
[27] $P432$	$3\mathbf{a},3\mathbf{b},3\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3}); \pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0); \pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$1a;6e;8g;12i$	$1b;6f;8g;12j$ $3\times8g;8\times24k$	$3c;6f;12h;12i;2\times24k$ $3\times12h;12\times24k$	$3d;6e;12h;12j;2\times24k$ $3\times12i;12\times24k$	$3\times6e;6\times24k$ $3\times12j;12\times24k$	$3\times6f;6\times24k$ $27\times24k$
[p^3] $P432$	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $p=\text{prime}>2;\ u,v,w=1,\dots,p-1$	$1a;\frac{p-1}{2}\times6e;\frac{p-1}{2}\times8g;\frac{p-1}{2}\times12i;\frac{p^3-13p+12}{24}\times24k$	$1b;\frac{p-1}{2}\times6f;\frac{p-1}{2}\times8g;\frac{p-1}{2}\times12j;\frac{p^3-13p+12}{24}\times24k$ $p\times8g;\frac{p(p^2-1)}{3}\times24k$	$3c;\frac{p-1}{2}\times6f;\frac{p-1}{2}\times12h;\frac{p-1}{2}\times12i;\frac{p^3-5p+4}{8}\times24k$ $p\times12h;\frac{p(p^2-1)}{2}\times24k$	$3d;\frac{p-1}{2}\times6e;\frac{p-1}{2}\times12h;\frac{p-1}{2}\times12j;\frac{p^3-5p+4}{8}\times24k$ $p\times12i;\frac{p(p^2-1)}{2}\times24k$	$p\times6e;\frac{p(p^2-1)}{4}\times24k$ $p\times12j;\frac{p(p^2-1)}{2}\times24k$	$p\times6f;\frac{p(p^2-1)}{4}\times24k$ $p^3\times24k$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 208, pp. 693–694.

O^2 No. 208 $P4_232$

	Axes	Coordinates	$2a$	$4b$ $12h$	$4c$ $12i$	$6d$ $12j$	$6e$ $12k$	$6f$ $12l$	$8g$ $24m$
I Maximal *translationengleiche* subgroups									
[2] $P23$ (195)			$1a;1b$	$4e$ $6f;6i$	$4e$ $2\times6g$	$3c;3d$ $2\times6h$	$6g$ $12j$	$6h$ $12j$	$2\times4e$ $2\times12j$
[4] $R32$ (155)	(rhombohedral axes)	$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$2c$	$1b;3e$ $2\times6f$	$1a;3d$ $2\times6f$	$6f$ $2\times6f$	$3d;3e$ $2\times3e;6f$	$3d;3e$ $2\times3d;6f$	$2c;6f$ $4\times6f$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y-z),\frac{1}{3}(x+y-2z),$ $\frac{1}{3}(x+y+z)+\frac{1}{4}$	$6c$	$3b;9e$ $2\times18f$	$3a;9d$ $2\times18f$	$18f$ $2\times18f$	$9d;9e$ $2\times9e;18f$	$9d;9e$ $2\times9d;18f$	$6c;18f$ $4\times18f$
conjugate:	$-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z),\frac{1}{3}(-x+y+2z),$ $\frac{1}{3}(-x+y-z)+\frac{1}{4}$							
conjugate:	$\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z),\frac{1}{3}(x-y+2z),$ $\frac{1}{3}(x-y-z)+\frac{1}{4}$							
conjugate:	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z),\frac{1}{3}(-x-y-2z),$ $\frac{1}{3}(-x-y+z)+\frac{1}{4}$							
[3] $P4_222$ (93)		$x+\frac{1}{2},y,z$	$2d$	$4o$ $4i;4j;4k$	$4n$ $4h;2\times4l$	$2a;2b;2c$ $4g;2\times4m$	$2f;4l$ $4o;8p$	$2e;4m$ $4n;8p$	$8p$ $3\times8p$
conjugate:	$\mathbf{b},\mathbf{c},\mathbf{a}$	$y+\frac{1}{2},z,x$							
conjugate:	$\mathbf{c},\mathbf{a},\mathbf{b}$	$z+\frac{1}{2},x,y$							
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**									
[2] $F4_132$ (210)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z;+(\frac{1}{2},0,0)$	$8a;8b$	$16c;16d$ $2\times48f$	$32e$ $96h$	$48f$ $96h$	$48g$ $2\times48g$	$48g$ $96h$	$2\times32e$ $2\times96h$
[2] $F4_132$ (210)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};+(\frac{1}{2},0,0)$	$8a;8b$	$32e$ $2\times48f$	$16c;16d$ $96h$	$48f$ $96h$	$48g$ $96h$	$48g$ $2\times48g$	$2\times32e$ $2\times96h$
[4] $I4_132$ (214)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z;+(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);+(0,0,\frac{1}{2})$	$16e$	$8a;24h$ $2\times48i$	$8b;24g$ $4\times24f$	$2\times24f$ $2\times48i$	$12c;12d;24f$ $2\times24h;48i$	$24g;24h$ $2\times24g;48i$	$16e;48i$ $4\times48i$
[4] $I4_132$ (214)	$2\mathbf{a},2\mathbf{b},2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4};+(\frac{1}{2},0,0);$ $+(0,\frac{1}{2},0);+(0,0,\frac{1}{2})$	$16e$	$8b;24g$ $2\times48i$	$8a;24h$ $2\times48i$	$2\times24f$ $4\times24f$	$24g;24h$ $2\times24g;48i$	$12c;12d;24f$ $2\times24h;48i$	$16e;48i$ $4\times48i$

	Axes	Coordinates	Wyckoff positions				
			$2a$	$4b$	$4c$	$6d$	$6e$
				$6f$	$8g$	$12h$	$12i$
				$12j$	$12k$	$12l$	$24m$
Enlarged unit cell, isomorphic							
[27] $P4_232$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$2a; 2\times 8g; 12h; 24m$	$4c; 8g; 2\times 12l; 3\times 24m$	$4b; 8g; 2\times 12k; 3\times 24m$	$6d; 12h; 12i; 12j; 5\times 24m$	$6e; 12i; 12k; 12l; 5\times 24m$
				$6f; 12j; 12k; 12l; 5\times 24m$	$3\times 8g; 8\times 24m$	$3\times 12h; 12\times 24m$	$3\times 12i; 12\times 24m$
				$3\times 12j; 12\times 24m$	$3\times 12l; 12\times 24m$	$3\times 12k; 12\times 24m$	$27\times 24m$
[p^3] $P4_232$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$; $u,v,w = 1,\ldots,p-1$	$2a$; $(p-1)\times 8g$; $\frac{p-1}{2}\times 12h$; $\frac{p^3-7p+6}{12}\times 24m$	$4b(c^*)$; $\frac{p-1}{2}\times 8g$; $(p-1)\times 12k(l^*)$; $\frac{p^3-4p+3}{6}\times 24m$	$4c(b^*)$; $\frac{p-1}{2}\times 8g$; $(p-1)\times 12l(k^*)$; $\frac{p^3-4p+3}{6}\times 24m$	$6d$; $\frac{p-1}{2}\times 12h$; $\frac{p-1}{2}\times 12i$; $\frac{p-1}{2}\times 12j$; $\frac{(p-1)^2(p+2)}{4}\times 24m$	$6e$; $\frac{p-1}{2}\times 12i$; $\frac{p-1}{2}\times 12k$; $\frac{p-1}{2}\times 12l$; $\frac{(p-1)^2(p+2)}{4}\times 24m$
				$6f$; $\frac{p-1}{2}\times 12j$; $\frac{p-1}{2}\times 12k$; $\frac{p-1}{2}\times 12l$; $\frac{(p-1)^2(p+2)}{4}\times 24m$	$p\times 8g$; $\frac{p(p^2-1)}{3}\times 24m$	$p\times 12h$; $\frac{p(p^2-1)}{2}\times 24m$	$p\times 12i$; $\frac{p(p^2-1)}{2}\times 24m$
				$p\times 12j$; $\frac{p(p^2-1)}{2}\times 24m$	$p\times 12k(l^*)$; $\frac{p(p^2-1)}{2}\times 24m$	$p\times 12l(k^*)$; $\frac{p(p^2-1)}{2}\times 24m$	$p^3\times 24m$

* $p = 4n-1$

O^3 No. 209 $F432$

Subgroup	Axes	Coordinates	4*a*	4*b*	8*c* 48*g*	24*d* 48*h*	24*e* 48*i*	32*f* 96*j*
I Maximal *translationengleiche* subgroups								
[2] $F23$ (196)			$4a$	$4b$	$4c; 4d$ $48h$	$24g$ $48h$	$24f$ $2\times24g$	$2\times16e$ $2\times48h$
[4] $R32$ (155)	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhombohedral axes)	$-x+y+z, x-y+z,$ $x+y-z$	$1a$	$1b$	$2c$ $2\times3d; 6f$	$3d; 3e$ $2\times3e; 6f$	$6f$ $2\times6f$	$2c; 6f$ $4\times6f$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(-\mathbf{b}+\mathbf{c})$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z)$, $\frac{2}{3}(-x-y+2z)$, $\frac{1}{3}(x+y+z)$	$3a$	$3b$	$6c$ $2\times9d; 18f$	$9d; 9e$ $2\times9e; 18f$	$18f$ $2\times18f$	$6c; 18f$ $4\times18f$
conjugate:	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(-\mathbf{b}-\mathbf{c})$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z)$, $\frac{2}{3}(x-y-2z)$, $\frac{1}{3}(-x+y-z)$						
conjugate:	$\frac{1}{2}(-\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{b}-\mathbf{c})$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z)$, $\frac{2}{3}(-x+y-2z)$, $\frac{1}{3}(x-y-z)$						
conjugate:	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z)$, $\frac{2}{3}(x+y+2z)$, $\frac{1}{3}(-x-y+z)$						
[3] $I422$ (97)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\mathbf{c}$	$x-y, x+y, z$	$2a$	$2b$	$4d$ $8h; 16k$	$4c; 8j$ $8i; 16k$	$4e; 8g$ $8f; 2\times8j$	$16k$ $3\times16k$
conjugate:	$\frac{1}{2}(\mathbf{b}-\mathbf{c})$, $\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $\mathbf{a}$	$y-z, y+z, x$						
conjugate:	$\frac{1}{2}(-\mathbf{a}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\mathbf{b}$	$-x+z, x+z, y$						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[4] $P4_232$ (208) 4 conjugate subgroups		$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$4b$	$4c$	$2a; 6d$ $2\times12k; 24m$	$6e; 6f; 12h$ $2\times12l; 24m$	$24m$ $2\times12h; 12i; 12j$	$8g; 24m$ $4\times24m$
[4] $P432$ (207) 4 conjugate subgroups			$1a; 3c$	$1b; 3d$	$8g$ $2\times12i; 24k$	$12i; 12j$ $2\times12j; 24k$	$6e; 6f; 12h$ $2\times24k$	$8g; 24k$ $4\times24k$
Enlarged unit cell, isomorphic								
[27] $F432$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$4a; 24e;$ $32f; 48g$	$4b; 24e;$ $32f; 48h$	$8c; 2\times32f;$ $48i; 96j$ $3\times48g;$ $12\times96j$	$24d; 48g; 48h;$ $48i; 5\times96j$ $3\times48h;$ $12\times96j$	$3\times24e; 6\times96j$ $3\times48i;$ $12\times96j$	$3\times32f;$ $8\times96j$ $27\times96j$
$[p^3]$ $F432$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$ $u, v, w = 1, \ldots, p-1$	$4a;$ $\frac{p-1}{2}\times24e;$ $\frac{p-1}{2}\times32f;$ $\frac{p-1}{2}\times48g;$ $\frac{p^3-13p+12}{24}\times96j$	$4b;$ $\frac{p-1}{2}\times24e;$ $\frac{p-1}{2}\times32f;$ $\frac{p-1}{2}\times48h;$ $\frac{p^3-13p+12}{24}\times96j$	$8c;$ $(p-1)\times32f;$ $\frac{p-1}{2}\times48i;$ $\frac{p^3-7p+6}{12}\times96j$ $p\times48g;$ $\frac{p(p^2-1)}{2}\times96j$	$24d;$ $\frac{p-1}{2}\times48g;$ $\frac{p-1}{2}\times48h;$ $\frac{p-1}{2}\times48i;$ $\frac{(p-1)^2(p+2)}{4}\times96j$ $p\times48h;$ $\frac{p(p^2-1)}{2}\times96j$	$p\times24e;$ $\frac{p(p^2-1)}{4}\times96j$ $p\times48i;$ $\frac{p(p^2-1)}{2}\times96j$	$p\times32f;$ $\frac{p(p^2-1)}{3}\times96j$ $p^3\times48h$

$F4_132$ No. 210 O^4

	Axes	Coordinates	Wyckoff positions $8a$	 $8b$	 $16c$	 $16d$	 $32e$ $48g$	 $48f$ $96h$
I Maximal *translationengleiche* subgroups								
[2] $F23$ (196)			$4a;4c$	$4b;4d$	$16e$	$16e$	$2\times16e$ $48h$	$24f;24g$ $2\times48h$
[4] $R32$ (155)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c}),$ $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhombohedral axes)	$-x+y+z-\frac{1}{8},$ $x-y+z-\frac{1}{8},$ $x+y-z-\frac{1}{8}$	$2c$	$2c$	$1a;3e$	$1b;3d$	$2c;6f$ $3d;3e;6f$	$2\times6f$ $4\times6f$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{a}+\mathbf{c}),$ $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)-\frac{1}{8}$	$6c$	$6c$	$3a;9e$	$3b;9d$	$6c;18f$ $9d;9e;18f$	$2\times18f$ $4\times18f$
conjugate:	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}-\mathbf{c}),$ $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z),$ $\frac{2}{3}(x-y-2z),$ $\frac{1}{3}(-x+y-z)-\frac{1}{8}$						
conjugate:	$\frac{1}{2}(-\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}-\mathbf{c}),$ $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z),$ $\frac{1}{3}(x-y-z)-\frac{1}{8}$						
conjugate:	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}+\mathbf{c}),$ $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z),$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)-\frac{1}{8}$						
[3] $I4_122$ (98)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x-y, x+y, z$	$4a$	$4b$	$8f$	$8f$	$16g$ $8f;16g$	$8c;8d;8e$ $3\times16g$
conjugate:	$\frac{1}{2}(\mathbf{b}-\mathbf{c}), \frac{1}{2}(\mathbf{b}+\mathbf{c}), \mathbf{a}$	$y-z, y+z, x$						
conjugate:	$\frac{1}{2}(-\mathbf{a}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c}), \mathbf{b}$	$-x+z, x+z, y$						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[4] $P4_132$ (213)	4 conjugate subgroups	$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$8c$	$8c$	$4a;12d$	$4b;12d$	$8c;24e$ $2\times12d;24e$	$2\times24e$ $4\times24e$
[4] $P4_332$ (212)	4 conjugate subgroups		$8c$	$8c$	$4a;12d$	$4b;12d$	$8c;24e$ $2\times12d;24e$	$2\times24e$ $4\times24e$
Enlarged unit cell, isomorphic								
[27] $F4_132$	$3\mathbf{b}, -3\mathbf{a}, 3\mathbf{c}$	$\frac{1}{3}y, -\frac{1}{3}x, \frac{1}{3}z;$ $\pm(\frac{1}{3},0,0);$ $\pm(0,\frac{1}{3},0);\pm(0,0,\frac{1}{3});$ $\pm(0,\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},0,\frac{1}{3});$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(0,\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},0,\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$8a;2\times32e;$ $48f;96h$	$8b;2\times32e;$ $48f;96h$	$16d;32e;$ $2\times48g;$ $3\times96h$	$16c;32e;$ $2\times48g;$ $3\times96h$	$3\times32e;$ $8\times96h$ $3\times48g;$ $12\times96h$	$3\times48f;$ $12\times96h$ $27\times96h$
[p^3] $F4_132$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ $p = \text{prime} = 4n+1$ $p\mathbf{b}, -p\mathbf{a}, p\mathbf{c}$ $p = \text{prime} = 4n-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z;$ $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $\frac{1}{p}y, -\frac{1}{p}x, \frac{1}{p}z;$ $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w = 1,\ldots,p-1$	$8a;$ $(p-1)\times32e;$ $\frac{p-1}{2}\times48f;$ $\frac{p^3-7p+6}{12}\times96h$	$8b;$ $(p-1)\times32e;$ $\frac{p-1}{2}\times48f;$ $\frac{p^3-7p+6}{12}\times96h$	$16c(d^*);$ $\frac{p-1}{2}\times32e;$ $(p-1)\times48g;$ $\frac{p^3-4p+3}{6}\times96h$	$16d(c^*);$ $\frac{p-1}{2}\times32e;$ $(p-1)\times48g;$ $\frac{p^3-4p+3}{6}\times96h$	$p\times32e;$ $\frac{p(p^2-1)}{3}\times96h$ $p\times48g;$ $\frac{p(p^2-1)}{2}\times96h$	$p\times48f;$ $\frac{p(p^2-1)}{2}\times96h$ $p^3\times96h$

* $p = 8n\pm3$

O^5 No. 211 $I432$

	Axes	Coordinates	Wyckoff positions $2a$	 $6b$	 $8c$ $24g$	 $12d$ $24h$	 $12e$ $24i$	 $16f$ $48j$
I Maximal *translationengleiche* subgroups								
[2] $I23$ (197)			$2a$	$6b$	$8c$ $2\times12e$	$12e$ $24f$	$12d$ $24f$	$2\times8c$ $2\times24f$
[4] $R32$ (155)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	$1a$	$3d$	$1b; 3e$ $2\times6f$	$2\times3e$ $2\times3d; 6f$	$6f$ $2\times3e; 6f$	$2c; 6f$ $4\times6f$
	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z)$, $\frac{1}{3}(-x-y+2z), \frac{2}{3}(x+y+z)$	$3a$	$9d$	$3b; 9e$ $2\times18f$	$2\times9e$ $2\times9d; 18f$	$18f$ $2\times9e; 18f$	$6c; 18f$ $4\times18f$
conjugate:	$\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z), \frac{1}{3}(x-y-2z)$, $\frac{2}{3}(-x+y-z)$						
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z), \frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$						
conjugate:	$\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z), \frac{1}{3}(x+y+2z)$, $\frac{2}{3}(-x-y+z)$						
[3] $I422$ (97)			$2a$	$2b; 4c$	$8j$ $8f; 2\times8i$	$4d; 8i$ $8g; 16k$	$4e; 8h$ $8j; 16k$	$16k$ $3\times16k$
conjugate:	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x						
conjugate:	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P4_232$ (208)			$2a$	$6d$	$4b; 4c$ $12i; 12j$	$6e; 6f$ $24m$	$12h$ $12k; 12l$	$2\times8g$ $2\times24m$
[2] $P432$ (207)			$1a; 1b$	$3c; 3d$	$8g$ $2\times12h$	$12h$ $12i; 12j$	$6e; 6f$ $24k$	$2\times8g$ $2\times24k$
Enlarged unit cell, isomorphic								
[27] $I432$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$2a; 12e$; $16f; 24h$	$6b; 12e; 24g$; $24h; 2\times48j$	$8c; 16f$; $2\times24i$; $3\times48j$ $3\times24g$; $12\times48j$	$12d; 24g$; $2\times24i$; $5\times48j$ $3\times24h$; $12\times48j$	$3\times12e$; $6\times48j$ $3\times24i$; $12\times48j$	$3\times16f$; $8\times48j$ $27\times48j$
$[p^3]$ $I432$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2$; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$2a$; $\frac{p-1}{2}\times12e$; $\frac{p-1}{2}\times16f$; $\frac{p-1}{2}\times24h$; $\frac{p^3-13p+12}{24}\times48j$	$6b$; $\frac{p-1}{2}\times12e$; $\frac{p-1}{2}\times24g$; $\frac{p-1}{2}\times24h$; $\frac{(p^3-5p+4)}{8}\times48j$	$8c$; $\frac{p-1}{2}\times16f$; $(p-1)\times24i$; $\frac{p^3-4p+3}{6}\times48j$ $p\times24g$; $\frac{p(p^2-1)}{2}\times48j$	$12d$; $\frac{p-1}{2}\times24g$; $(p-1)\times24i$; $\frac{(p-1)^2(p+2)}{4}\times48j$ $p\times24h$; $\frac{p(p^2-1)}{2}\times48j$	$p\times12e$; $\frac{p(p^2-1)}{4}\times48j$ $p\times24i$; $\frac{p(p^2-1)}{2}\times48j$	$p\times16f$; $\frac{p(p^2-1)}{3}\times48j$ $p^3\times48j$

$P4_332$ No. 212 O^6

	Axes	Coordinates	Wyckoff positions 4a	4b	8c	12d	24e
I Maximal *translationengleiche* subgroups							
[2] $P2_13$ (198)			$4a$	$4a$	$2\times4a$	$12b$	$2\times12b$
[4] $R32$ (155)	(rhombohedral axes)	$x-\frac{1}{8}, y-\frac{1}{8}, z-\frac{1}{8}$	$1a; 3e$	$1b; 3d$	$2c; 6f$	$3d; 3e; 6f$	$4\times6f$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)-\frac{1}{8}$	$3a; 9e$	$3b; 9d$	$6c; 18f$	$9d; 9e; 18f$	$4\times18f$
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)-\frac{1}{2}$, $\frac{1}{3}(-x+y-z)-\frac{1}{8}$					
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x+y+z)-\frac{1}{2}$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)-\frac{1}{8}$					
	conjugate: $-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}$, $\frac{1}{3}(-x-y-2z)+\frac{1}{2}$, $\frac{1}{3}(-x-y+z)-\frac{1}{8}$					
[3] $P4_32_12$ (96)		$x-\frac{1}{4}, y, z+\frac{1}{8}$	$4a$	$4a$	$8b$	$4a; 8b$	$3\times8b$
	conjugate: $\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y-\frac{1}{4}, z, x+\frac{1}{8}$					
	conjugate: $\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z-\frac{1}{4}, x, y+\frac{1}{8}$					
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[27] $P4_132$ (213)	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$4a; 8c; 2\times12d$; $3\times24e$	$4b; 8c; 2\times12d$; $3\times24e$	$3\times8c; 8\times24e$	$3\times12d$; $12\times24e$	$27\times24e$
$[p^3]$ $P4_132$ (213)	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime $= 4n-1$;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w = 1,\ldots,p-1$	$4a(b^*)$; $\frac{p-1}{2}\times8c$; $(p-1)\times12d$; $\frac{p^3-4p+3}{6}\times24e$	$4b(a^*)$; $\frac{p-1}{2}\times8c$; $(p-1)\times12d$; $\frac{p^3-4p+3}{6}\times24e$	$p\times8c$; $\frac{p(p^2-1)}{3}\times24e$	$p\times12d$; $\frac{p(p^2-1)}{2}\times24e$	$p^3\times24e$
$[p^3]$ $P4_332$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime $= 4n+1$;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w = 1,\ldots,p-1$	$4a(b^\dagger)$; $\frac{p-1}{2}\times8c$; $(p-1)\times12d$; $\frac{p^3-4p+3}{6}\times24e$	$4b(a^\dagger)$; $\frac{p-1}{2}\times8c$; $(p-1)\times12d$; $\frac{p^3-4p+3}{6}\times24e$	$p\times8c$; $\frac{p(p^2-1)}{3}\times24e$	$p\times12d$; $\frac{p(p^2-1)}{2}\times24e$	$p^3\times24e$

* $p = 8n-1$ † $p = 8n+5$

O^7 No. 213 $P4_132$

	Axes	Coordinates	4a	4b	8c	12d	24e
I Maximal *translationengleiche* subgroups							
[2] $P2_13$ (198)			$4a$	$4a$	$2\times 4a$	$12b$	$2\times 12b$
[4] $R32$ (155)	(rhombohedral axes)	$x-\frac{3}{8}, y-\frac{3}{8}, z-\frac{3}{8}$	$1a; 3e$	$1b; 3d$	$2c; 6f$	$3d; 3e; 6f$	$4\times 6f$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)-\frac{3}{8}$	$3a; 9e$	$3b; 9d$	$6c; 18f$	$9d; 9e; 18f$	$4\times 18f$
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)-\frac{1}{2}$, $\frac{1}{3}(-x+y-z)-\frac{3}{8}$					
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x+y+z)-\frac{1}{2}$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)-\frac{3}{8}$					
	conjugate: $-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}$, $\frac{1}{3}(-x-y-2z)+\frac{1}{2}$, $\frac{1}{3}(-x-y+z)-\frac{3}{8}$					
[3] $P4_12_12$ (92)		$x+\frac{1}{4}, y, z-\frac{1}{8}$	$4a$	$4a$	$8b$	$4a; 8b$	$3\times 8b$
	conjugate: $\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y+\frac{1}{4}, z, x-\frac{1}{8}$					
	conjugate: $\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z+\frac{1}{4}, x, y-\frac{1}{8}$					
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[27] $P4_332$ (212)	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3}); \pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0); \pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$4a; 8c; 2\times 12d; 3\times 24e$	$4b; 8c; 2\times 12d; 3\times 24e$	$3\times 8c; 8\times 24e$	$3\times 12d; 12\times 24e$	$27\times 24e$
[p^3] $P4_132$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime = $4n+1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$; $u,v,w = 1,\ldots,p-1$	$4a(b^*); \frac{p-1}{2}\times 8c; (p-1)\times 12d; \frac{p^3-4p+3}{6}\times 24e$	$4b(a^*); \frac{p-1}{2}\times 8c; (p-1)\times 12d; \frac{p^3-4p+3}{6}\times 24e$	$p\times 8c; \frac{p(p^2-1)}{3}\times 24e$	$p\times 12d; \frac{p(p^2-1)}{2}\times 24e$	$p^3\times 24e$
[p^3] $P4_332$ (212)	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime = $4n-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$; $u,v,w = 1,\ldots,p-1$	$4a(b^\dagger); \frac{p-1}{2}\times 8c; (p-1)\times 12d; \frac{p^3-4p+3}{6}\times 24e$	$4b(a^\dagger); \frac{p-1}{2}\times 8c; (p-1)\times 12d; \frac{p^3-4p+3}{6}\times 24e$	$p\times 8c; \frac{p(p^2-1)}{3}\times 24e$	$p\times 12d; \frac{p(p^2-1)}{2}\times 24e$	$p^3\times 24e$

* $p = 8n+5$ † $p = 8n-1$

$I4_132$ No. 214 O^8

	Axes	Coordinates	Wyckoff positions $8a$	 $8b$	 $12c$	 $12d$ $24g$	 $16e$ $24h$	 $24f$ $48i$
I Maximal *translationengleiche* subgroups								
[2] $I2_13$ (199)			$8a$	$8a$	$12b$	$12b$ $24c$	$2\times 8a$ $24c$	$2\times 12b$ $2\times 24c$
[4] $R32$ (155)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z-\frac{1}{4}, x+z-\frac{1}{4}, x+y-\frac{1}{4}$ (rhombohedral axes)	$1a; 3d$	$1b; 3e$	$3d; 3e$	$3d; 3e$ $2\times 3e; 6f$	$2c; 6f$ $2\times 3d; 6f$	$2\times 6f$ $4\times 6f$
	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z), \frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)-\frac{1}{4}$	$3a; 9d$	$3b; 9e$	$9d; 9e$	$9d; 9e$ $2\times 9e; 18f$	$6c; 18f$ $2\times 9d; 18f$	$2\times 18f$ $4\times 18f$
conjugate:	$\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z), \frac{1}{3}(x-y-2z)+\frac{1}{2}$, $\frac{2}{3}(-x+y-z)-\frac{1}{4}$						
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z)+\frac{1}{2}, \frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)-\frac{1}{4}$						
conjugate:	$\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z)+\frac{1}{2}, \frac{1}{3}(x+y+2z)+\frac{1}{2}$, $\frac{2}{3}(-x-y+z)-\frac{1}{4}$						
[3] $I4_122$ (98)		$x, y-\frac{1}{4}, z-\frac{1}{8}$	$8e$	$8d$	$4a; 8f$	$4b; 8f$ $8d; 16g$	$16g$ $8e; 16g$	$8c; 2\times 8f$ $3\times 16g$
conjugate:	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y, z-\frac{1}{4}, x-\frac{1}{8}$						
conjugate:	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z, x-\frac{1}{4}, y-\frac{1}{8}$						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P4_132$ (213)			$8c$	$4a; 4b$	$12d$	$12d$ $2\times 12d$	$2\times 8c$ $24e$	$24e$ $2\times 24e$
[2] $P4_332$ (212)			$4a; 4b$	$8c$	$12d$	$12d$ $24e$	$2\times 8c$ $2\times 12d$	$24e$ $2\times 24e$
Enlarged unit cell, isomorphic								
[27] $I4_132$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0); \pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$8b; 16e$; $2\times 24g$; $3\times 48i$	$8a; 16e$; $2\times 24h$; $3\times 48i$	$12c; 24f$; $24g; 24h$; $5\times 48i$	$12d; 24f$; $24g; 24h$; $5\times 48i$ $3\times 24h$; $12\times 48i$	$3\times 16e$; $8\times 48i$ $3\times 24g$; $12\times 48i$	$3\times 24f$; $12\times 48i$ $27\times 48i$
[p^3] $I4_132$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ p = prime > 2; $u,v,w = 1,\ldots,p-1$	$8a(b^*)$; $\frac{p-1}{2}\times 16e$; $(p-1)\times$ $24h(g^*)$; $\frac{p^3-4p+3}{6}\times$ $48i$	$8b(a^*)$; $\frac{p-1}{2}\times 16e$; $(p-1)\times$ $24g(h^*)$; $\frac{p^3-4p+3}{6}\times$ $48i$	$12c(d^\dagger)$; $\frac{p-1}{2}\times 24f$; $\frac{p-1}{2}\times 24g$; $\frac{p-1}{2}\times 24h$; $\frac{(p-1)^2(p+2)}{4}\times$ $48i$	$12d(c^\dagger)$; $\frac{p-1}{2}\times 24f$; $\frac{p-1}{2}\times 24g$; $\frac{p-1}{2}\times 24h$; $\frac{(p-1)^2(p+2)}{4}\times$ $48i$ $p\times 24g(h^*)$; $\frac{p(p^2-1)}{2}\times 48i$	$p\times 16e$; $\frac{p(p^2-1)}{3}\times 48i$ $p\times 24h(g^*)$; $\frac{p(p^2-1)}{2}\times 48i$	$p\times 24f$; $\frac{p(p^2-1)}{2}\times 48i$ $p^3\times 48i$

* $p = 4n-1$ † $p = 8n+5$ or $p = 8n+7$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 215, pp. 701–702.

T_d^1 No. 215 $P\bar{4}3m$

	Axes	Coordinates	Wyckoff positions $1a$	$1b$	$3c$	$3d$	$4e$	$6f$	$6g$ $12i$	$12h$ $24j$
I Maximal *translationengleiche* subgroups										
[2] $P23$ (195)			$1a$	$1b$	$3c$	$3d$	$4e$	$6f$	$6i$ $12j$	$6g; 6h$ $2\times 12j$
[4] $R3m$ (160)	(rhombohedral axes)		$1a$	$1a$	$3b$	$3b$	$1a; 3b$	$2\times 3b$	$2\times 3b$ $2\times 3b; 6c$	$2\times 6c$ $4\times 6c$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y-z), \frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$3a$	$3a$	$9b$	$9b$	$3a; 9b$	$2\times 9b$	$2\times 9b$ $2\times 9b; 18c$	$2\times 18c$ $4\times 18c$
conjugate:	$-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z), \frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)$								
conjugate:	$\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z), \frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)$								
conjugate:	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z), \frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$								
[3] $P\bar{4}2m$ (111)			$1a$	$1b$	$1d; 2f$	$1c; 2e$	$4n$	$2g; 4i$	$2h; 4j$ $4n; 8o$	$4k; 4l; 4m$ $3\times 8o$
conjugate:	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x								
conjugate:	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y								
II Maximal *klassengleiche* subgroups **Enlarged unit cell, non-isomorphic**										
[2] $F\bar{4}3c$ (219)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z; +(\frac{1}{2},0,0)$	$8a$	$8b$	$24c$	$24d$	$32e$	$48f$	$48g$ $96h$	$96h$ $2\times 96h$
[2] $F\bar{4}3m$ (216)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z; +(\frac{1}{2},0,0)$	$4a; 4b$	$4c; 4d$	$24g$	$24f$	$2\times 16e$	$2\times 24f$	$2\times 24g$ $2\times 48h$	$96i$ $2\times 96i$
[4] $I\bar{4}3m$ (217)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z; +(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0); +(0,0,\frac{1}{2})$	$2a; 6b$	$8c$	$24g$	$12d; 12e$	$8c; 24g$	$2\times 12e; 24f$	$2\times 24g$ $2\times 24g; 48h$	$2\times 48h$ $4\times 48h$
[4] $I\bar{4}3m$ (217)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0); +(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$8c$	$2a; 6b$	$12d; 12e$	$24g$	$8c; 24g$	$2\times 24g$	$2\times 12e; 24f$ $2\times 24g; 48h$	$2\times 48h$ $4\times 48h$

	Axes	Coordinates	Wyckoff positions					
			$1a$	$1b$	$3c$ $6g$	$3d$ $12h$	$4e$ $12i$	$6f$ $24j$
Enlarged unit cell, isomorphic								
$[27]\,P\bar{4}3m$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3}); \pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0); \pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$1a; 2\times4e; 6f; 12i$	$1b; 2\times4e; 6g; 12i$	$3c; 6g; 12h; 3\times12i; 24j$	$3d; 6f; 12h; 3\times12i; 24j$	$3\times4e; 6\times12i; 24j$	$3\times6f; 6\times12i; 3\times24j$
					$3\times6g; 6\times12i; 3\times24j$	$3\times12h; 12\times24j$	$9\times12i; 9\times24j$	$27\times24j$
$[p^3]\,P\bar{4}3m$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2$;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w = 1,\ldots,p-1$	$1a; (p-1)\times4e; \frac{p-1}{2}\times6f; \frac{(p-1)(p-2)}{2}\times12i; \frac{(p-1)(p-2)(p-3)}{24}\times24j$	$1b; (p-1)\times4e; \frac{p-1}{2}\times6g; \frac{(p-1)(p-2)}{2}\times12i; \frac{(p-1)(p-2)(p-3)}{24}\times24j$	$3c; \frac{p-1}{2}\times6g; \frac{p-1}{2}\times12h; \frac{p(p-1)}{2}\times12i; \frac{(p^2-1)(p-2)}{8}\times24j$	$3d; \frac{p-1}{2}\times6f; \frac{p-1}{2}\times12h; \frac{p(p-1)}{2}\times12i; \frac{(p^2-1)(p-2)}{8}\times24j$	$p\times4e; p(p-1)\times12i; \frac{p(p-1)(p-2)}{6}\times24j$	$p\times6f; p(p-1)\times12i; \frac{p(p-1)^2}{4}\times24j$
					$p\times6g; p(p-1)\times12i; \frac{p(p-1)^2}{4}\times24j$	$p\times12h; \frac{p(p^2-1)}{2}\times24j$	$p^2\times12i; \frac{p^2(p-1)}{2}\times24j$	$p^3\times24j$

T_d^2 No. 216 $F\bar{4}3m$

	Axes	Coordinates	Wyckoff positions					
			$4a$	$4b$	$4c$	$4d$ $24g$	$16e$ $48h$	$24f$ $96i$
I Maximal *translationengleiche* subgroups								
[2] $F23$ (196)			$4a$	$4b$	$4c$	$4d$ $24g$	$16e$ $48h$	$24f$ $2{\times}48h$
[4] $R3m$ (160)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}+\mathbf{c}),$ $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhombohedral axes)	$-x+y+z, x-y+z,$ $x+y-z$	$1a$	$1a$	$1a$	$1a$ $2{\times}3b$	$1a; 3b$ $2{\times}3b; 6c$	$2{\times}3b$ $4{\times}6c$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}+\mathbf{c}),$ $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)$	$3a$	$3a$	$3a$	$3a$ $2{\times}9b$	$3a; 9b$ $2{\times}9b; 18c$	$2{\times}9b$ $4{\times}18c$
	conjugate: $\frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}(-\mathbf{b}-\mathbf{c}),$ $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z),$ $\frac{2}{3}(x-y-2z),$ $\frac{1}{3}(-x+y-z)$						
	conjugate: $\frac{1}{2}(-\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}-\mathbf{c}),$ $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z),$ $\frac{1}{3}(x-y-z)$						
	conjugate: $\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{b}+\mathbf{c}),$ $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z),$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)$						
[3] $I\bar{4}m2$ (119)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \mathbf{c}$	$x-y, x+y, z$	$2a$	$2b$	$2c$	$2d$ $4f; 8h$	$8i$ $8i; 16j$	$4e; 8g$ $3{\times}16j$
	conjugate: $\frac{1}{2}(\mathbf{b}-\mathbf{c}),\ \frac{1}{2}(\mathbf{b}+\mathbf{c}),\ \mathbf{a}$	$y-z, y+z, x$						
	conjugate: $\frac{1}{2}(-\mathbf{a}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c}), \mathbf{b}$	$-x+z, x+z, y$						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[4] $P\bar{4}3m$ (215)	4 conjugate subgroups		$1a; 3c$	$1b; 3d$	$4e$	$4e$ $2{\times}12i$	$4e; 12i$ $2{\times}12i; 24j$	$6f; 6g; 12h$ $4{\times}24j$
[4] $P\bar{4}3m$ (215)	4 conjugate subgroups	$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$4e$	$4e$	$1b; 3d$	$1a; 3c$ $6f; 6g; 12h$	$4e; 12i$ $2{\times}12i; 24j$	$2{\times}12i$ $4{\times}24j$
Enlarged unit cell, isomorphic								
[27] $F\bar{4}3m$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$4a; 2{\times}16e;$ $24f; 48h$	$4b; 2{\times}16e;$ $24f; 48h$	$4d; 2{\times}16e;$ $24g; 48h$	$4c; 2{\times}16e;$ $24g; 48h$ $3{\times}24g;$ $6{\times}48h;$ $3{\times}96i$	$3{\times}16e;$ $6{\times}48h; 96i$ $9{\times}48h;$ $9{\times}96i$	$3{\times}24f;$ $6{\times}48h;$ $3{\times}96i$ $27{\times}96i$
[p^3] $F\bar{4}3m$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w = 1,\ldots,p-1$	$4a;$ $(p-1){\times}16e;$ $\frac{p-1}{2}{\times}24f;$ $\frac{(p-1)(p-2)}{2}{\times}$ $48h;$ $\frac{(p-1)(p-2)(p-3)}{24}{\times}96i$	$4b;$ $(p-1){\times}16e;$ $\frac{p-1}{2}{\times}24f;$ $\frac{(p-1)(p-2)}{2}{\times}$ $48h;$ $\frac{(p-1)(p-2)(p-3)}{24}{\times}96i$	$4c(d^*);$ $(p-1){\times}16e;$ $\frac{p-1}{2}{\times}24g;$ $\frac{(p-1)(p-2)}{2}{\times}$ $48h;$ $\frac{(p-1)(p-2)(p-3)}{24}{\times}96i$	$4d(c^*);$ $(p-1){\times}16e;$ $\frac{p-1}{2}{\times}24g;$ $\frac{(p-1)(p-2)}{2}{\times}$ $48h;$ $\frac{(p-1)(p-2)(p-3)}{24}{\times}96i$ $p{\times}24g;$ $p(p-1){\times}48h;$ $\frac{p(p-1)^2}{4}{\times}96i$	$p{\times}16e;$ $p(p-1){\times}$ $48h;$ $\frac{p(p-1)(p-2)}{6}{\times}96i$ $p^2{\times}48h;$ $\frac{p^2(p-1)}{2}{\times}96i$	$p{\times}24f;$ $p(p-1){\times}$ $48h;$ $\frac{p(p-1)^2}{4}{\times}$ $96i$ $p^3{\times}96i$

* $p = 4n-1$

$I\bar{4}3m$ No. 217 T_d^3

	Axes	Coordinates	Wyckoff positions					
			$2a$	$6b$	$8c$	$12d$	$12e$ $24g$	$24f$ $48h$
I Maximal *translationengleiche* subgroups								
[2] $I23$ (197)			$2a$	$6b$	$8c$	$12e$	$12d$ $24f$	$2\times12e$ $2\times24f$
[4] $R3m$ (160)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	$1a$	$3b$	$1a; 3b$	$6c$	$2\times3b$ $2\times3b; 6c$	$2\times6c$ $4\times6c$
	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hex. axes)	$\frac{1}{3}(-2x+y+z)$, $\frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)$	$3a$	$9b$	$3a; 9b$	$18c$	$2\times9b$ $2\times9b; 18c$	$2\times18c$ $4\times18c$
	conjugate: $\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hex. axes)	$\frac{1}{3}(2x+y-z)$, $\frac{1}{3}(x-y-2z)$, $\frac{2}{3}(-x+y-z)$						
	conjugate: $-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hex. axes)	$\frac{1}{3}(-2x-y-z)$, $\frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$						
	conjugate: $\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hex. axes)	$\frac{1}{3}(2x-y+z)$, $\frac{1}{3}(x+y+2z)$, $\frac{2}{3}(-x-y+z)$						
[3] $I\bar{4}2m$ (121)			$2a$	$2b; 4c$	$8i$	$4d; 8g$	$4e; 8f$ $8i; 16j$	$2\times8g; 8h$ $3\times16j$
	conjugate: $\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x						
	conjugate: $\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[2] $P\bar{4}3n$ (218)			$2a$	$6b$	$8e$	$6c; 6d$	$12f$ $24i$	$12g; 12h$ $2\times24i$
[2] $P\bar{4}3m$ (215)			$1a; 1b$	$3c; 3d$	$2\times4e$	$12h$	$6f; 6g$ $2\times12i$	$2\times12h$ $2\times24j$
Enlarged unit cell, isomorphic								
[27] $I\bar{4}3m$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$2a; 2\times8c; 12e; 24g$	$6b; 12e; 24f; 3\times24g; 48h$	$3\times8c; 6\times24g; 48h$	$12d; 24f; 6\times48h$	$3\times12e; 6\times24g; 3\times48h$ $9\times24g; 9\times48h$	$3\times24f; 12\times48h$ $27\times48h$
$[p^3]$ $I\bar{4}3m$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$2a$; $(p-1)\times8c$; $\frac{p-1}{2}\times12e$; $\frac{(p-1)(p-2)}{2}\times24g$; $\frac{(p-1)(p-2)(p-3)}{24}\times48h$	$6b$; $\frac{p-1}{2}\times12e$; $\frac{p-1}{2}\times24f$; $\frac{p(p-1)}{2}\times24g$; $\frac{(p^2-1)(p-2)}{8}\times48h$	$p\times8c$; $p(p-1)\times24g$; $\frac{p(p-1)(p-2)}{6}\times48h$	$12d$; $\frac{p-1}{2}\times24f$; $\frac{p(p^2-1)}{4}\times48h$	$p\times12e$; $p(p-1)\times24g$; $\frac{p(p-1)^2}{4}\times48h$ $p^2\times24g$; $\frac{p^2(p-1)}{2}\times48h$	$p\times24f$; $\frac{p(p^2-1)}{2}\times48h$ $p^3\times48h$

T_d^4 No. 218 $P\bar{4}3n$

	Axes	Coordinates	Wyckoff positions $2a$	 $6b$	 $6c$	 $6d$ $12g$	 $8e$ $12h$	 $12f$ $24i$
I Maximal *translationengleiche* subgroups								
[2] $P23$ (195)			$1a;1b$	$3c;3d$	$6h$	$6g$ $2\times6h$	$2\times4e$ $2\times6g$	$6f;6i$ $2\times12j$
[4] $R3c$ (161)	(rhombohedral axes)		$2a$	$6b$	$6b$	$6b$ $2\times6b$	$2a;6b$ $2\times6b$	$2\times6b$ $4\times6b$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y-z), \frac{1}{3}(x+y-2z), \frac{1}{3}(x+y+z)$	$6a$	$18b$	$18b$	$18b$ $2\times18b$	$6a;18b$ $2\times18b$	$2\times18b$ $4\times18b$
conjugate:	$-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z), \frac{1}{3}(-x+y+2z), \frac{1}{3}(-x+y-z)$						
conjugate:	$\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z), \frac{1}{3}(x-y+2z), \frac{1}{3}(x-y-z)$						
conjugate:	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z), \frac{1}{3}(-x-y-2z), \frac{1}{3}(-x-y+z)$						
[3] $P\bar{4}2c$ (112)		$x+\frac{1}{2}, y, z+\frac{1}{4}$	$2b$	$2a;2c;2d$	$2e;4i$	$2f;4j$ $2\times4i;4k$	$8n$ $2\times4j;4l$	$4g;4h;4m$ $3\times8n$
conjugate:	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y+\frac{1}{2}, z, x+\frac{1}{4}$						
conjugate:	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z+\frac{1}{2}, x, y+\frac{1}{4}$						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, non-isomorphic								
[4] $I\bar{4}3d$ (220)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(0,0,\frac{1}{2})$	$16c$	$2\times24d$	$48e$	$12a;12b;24d$ $2\times48e$	$16c;48e$ $4\times24d$	$2\times48e$ $4\times48e$
[4] $I\bar{4}3d$ (220)	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}; +(\frac{1}{2},0,0); +(0,\frac{1}{2},0); +(0,0,\frac{1}{2})$	$16c$	$2\times24d$	$12a;12b;24d$	$48e$ $4\times24d$	$16c;48e$ $2\times48e$	$2\times48e$ $4\times48e$
Enlarged unit cell, isomorphic								
[27] $P\bar{4}3n$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z; \pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3}); \pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},0); \pm(0,\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0); \pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{2}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$2a;2\times8e;$ $12f;24i$	$6b;12f;12g;$ $12h;5\times24i$	$6c;12g;$ $6\times24i$	$6d;12h;$ $6\times24i$ $3\times12g;$ $12\times24i$	$3\times8e;$ $8\times24i$ $3\times12h;$ $12\times24i$	$3\times12f;$ $12\times24i$ $27\times24i$
[p^3] $P\bar{4}3n$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z; +(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ p = prime > 4; $u,v,w = 1,\ldots,p-1$	$2a;$ $(p-1)\times8e;$ $\frac{p-1}{2}\times12f;$ $\frac{p^3-7p+6}{12}\times24i$	$6b;\frac{p-1}{2}\times12f;$ $\frac{p-1}{2}\times12g;$ $\frac{p-1}{2}\times12h;$ $\frac{(p-1)^2(p+2)}{4}\times24i$	$6c;$ $\frac{p-1}{2}\times12g;$ $\frac{p(p^2-1)}{4}\times24i$	$6d;$ $\frac{p-1}{2}\times12h;$ $\frac{p(p^2-1)}{4}\times24i$ $p\times12g;$ $\frac{p(p^2-1)}{2}\times24i$	$p\times8e;$ $\frac{p(p^2-1)}{3}\times24i$ $p\times12h;$ $\frac{p(p^2-1)}{2}\times24i$	$p\times12f;$ $\frac{p(p^2-1)}{2}\times24i$ $p^3\times24i$

$F\bar{4}3c$ No. 219 T_d^5

	Axes	Coordinates	Wyckoff positions					
			$8a$	$8b$	$24c$	$24d$	$32e$ $48g$	$48f$ $96h$
I Maximal *translationengleiche* subgroups								
[2] $F23$ (196)			$4a;4b$	$4c;4d$	$24g$	$24f$	$2\times16e$ $2\times24g$	$2\times24f$ $2\times48h$
[4] $R3c$ (161)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}),\frac{1}{2}(\mathbf{a}+\mathbf{c}),$ $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhombohedral axes)	$-x+y+z,x-y+z,$ $x+y-z$	$2a$	$2a$	$6b$	$6b$	$2a;6b$ $2\times6b$	$2\times6b$ $4\times6b$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}),\frac{1}{2}(-\mathbf{b}+\mathbf{c}),$ $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)$	$6a$	$6a$	$18b$	$18b$	$6a;18b$ $2\times18b$	$2\times18b$ $4\times18b$
	conjugate: $\frac{1}{2}(\mathbf{a}+\mathbf{b}),\frac{1}{2}(-\mathbf{b}-\mathbf{c}),$ $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z),$ $\frac{2}{3}(x-y-2z),$ $\frac{1}{3}(-x+y-z)$						
	conjugate: $\frac{1}{2}(-\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{b}-\mathbf{c}),$ $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z),$ $\frac{1}{3}(x-y-z)$						
	conjugate: $\frac{1}{2}(\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{b}+\mathbf{c}),$ $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z),$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)$						
[3] $I\bar{4}c2$ (120)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{a}+\mathbf{b}),\mathbf{c}$	$x-y,x+y,z+\frac{1}{4}$	$4a$	$4d$	$4c;8h$	$4b;8e$	$16i$ $8g;2\times8h$	$2\times8e;8f$ $3\times16i$
	conjugate: $\frac{1}{2}(\mathbf{b}-\mathbf{c}),\frac{1}{2}(\mathbf{b}+\mathbf{c}),\mathbf{a}$	$y-z,y+z,x+\frac{1}{4}$						
	conjugate: $\frac{1}{2}(-\mathbf{a}+\mathbf{c}),\frac{1}{2}(\mathbf{a}+\mathbf{c}),\mathbf{b}$	$-x+z,x+z,y+\frac{1}{4}$						
II Maximal *klassengleiche* subgroups								
Loss of centring translations								
[4] $P\bar{4}3n$ (218)	4 conjugate subgroups		$2a;6b$	$8e$	$24i$	$6c;6d;12f$	$8e;24i$ $2\times24i$	$2\times12f;12g;12h$ $4\times24i$
[4] $P\bar{4}3n$ (218)	4 conjugate subgroups	$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$8e$	$2a;6b$	$6c;6d;12f$	$24i$	$8e;24i$ $2\times12f;12g;$ $12h$	$2\times24i$ $4\times24i$
Enlarged unit cell, isomorphic								
[27] $F\bar{4}3c$	$3\mathbf{a},3\mathbf{b},3\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z;\ \pm(\frac{1}{3},0,0);$ $\pm(0,\frac{1}{3},0);\pm(0,0,\frac{1}{3});$ $\pm(0,\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},0,\frac{1}{3});$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(0,\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},0,\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$8a;2\times32e;$ $48f;96h$	$8b;2\times32e;$ $48g;96h$	$24c;48g;$ $6\times96h$	$24d;48f;$ $6\times96h$	$3\times32e;$ $8\times96h$ $3\times48g;$ $12\times96h$	$3\times48f;$ $12\times96h$ $27\times96h$
$[p^3]$ $F\bar{4}3c$	$p\mathbf{a},p\mathbf{b},p\mathbf{c}$ p = prime >2; $u,v,w=1,\dots,p-1$	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z;+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$8a;$ $(p-1)\times32e;$ $\frac{p-1}{2}\times48f;$ $\frac{p^3-7p+6}{12}\times$ $96h$	$8b;$ $(p-1)\times32e;$ $\frac{p-1}{2}\times48g;$ $\frac{p^3-7p+6}{12}\times$ $96h$	$24c;$ $\frac{p-1}{2}\times48g;$ $\frac{p(p^2-1)}{4}\times$ $96h$	$24d;$ $\frac{p-1}{2}\times48f;$ $\frac{p(p^2-1)}{4}\times$ $96h$	$p\times32e;$ $\frac{p(p^2-1)}{3}\times96h$ $p\times48g;$ $\frac{p(p^2-1)}{2}\times96h$	$p\times48f;$ $\frac{p(p^2-1)}{2}\times96h$ $p^3\times96h$

T_d^6 No. 220 $I\bar{4}3d$

	Axes	Coordinates	12a	12b	16c	24d	48e
I Maximal *translationengleiche* subgroups							
[2] $I2_13$ (199)			12b	12b	2×8a	2×12b	2×24c
[4] $R3c$ (161)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	6b	6b	2a; 6b	2×6b	4×6b
	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z), \frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)$	18b	18b	6a; 18b	2×18b	4×18b
conjugate:	$\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z)$, $\frac{1}{3}(x-y-2z)+\frac{1}{2}$, $\frac{2}{3}(-x+y-z)$					
conjugate:	$-\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$					
conjugate:	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z)-\frac{1}{2}$, $\frac{1}{3}(x+y+2z)-\frac{1}{2}$, $\frac{2}{3}(-x-y+z)$					
[3] $I\bar{4}2d$ (122)		$x, y+\frac{1}{4}, z-\frac{1}{8}$	4a; 8d	4b; 8d	16e	8c; 2×8d	3×16e
conjugate:	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	$y, z+\frac{1}{4}, x-\frac{1}{8}$					
conjugate:	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	$z, x+\frac{1}{4}, y-\frac{1}{8}$					
II Maximal *klassengleiche* subgroups							
Enlarged unit cell, isomorphic							
[27] $I\bar{4}3d$	3$\mathbf{a}$, 3$\mathbf{b}$, 3$\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	12a; 24d; 6×48e	12b; 24d; 6×48e	3×16c; 8×48e	3×24d; 12×48e	27×48e
$[p^3]$ $I\bar{4}3d$	$p\mathbf{a}$, $p\mathbf{b}$, $p\mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ p = prime > 2; $u, v, w = 1, \ldots, p-1$	12$a(b^*)$; $\frac{p-1}{2}$×24d; $\frac{p(p^2-1)}{4}$×48e	12$b(a^*)$; $\frac{p-1}{2}$×24d; $\frac{p(p^2-1)}{4}$×48e	p×16c; $\frac{p(p^2-1)}{3}$×48e	p×24d; $\frac{p(p^2-1)}{2}$×48e	p^3×48e

* $p = 8n+5$ or $p = 8n+7$

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 221, pp. 708–709.

$Pm\bar{3}m$ No. 221 $P4/m\bar{3}2/m$ O_h^1

	Axes	Coordinates	Wyckoff positions						
			$1a$	$1b$	$3c$	$3d$	$6e$	$6f$	$8g$
			$12h$	$12i$	$12j$	$24k$	$24l$	$24m$	$48n$

I Maximal *translationengleiche* subgroups

[2] $P\bar{4}3m$			$1a$	$1b$	$3c$	$3d$	$6f$	$6g$	$2\times 4e$
(215)			$12h$	$12i$	$12i$	$24j$	$24j$	$2\times 12i$	$2\times 24j$
[2] $P432$			$1a$	$1b$	$3c$	$3d$	$6e$	$6f$	$8g$
(207)			$12h$	$12i$	$12j$	$24k$	$24k$	$24k$	$2\times 24k$
[2] $Pm\bar{3}$			$1a$	$1b$	$3c$	$3d$	$6e$	$6h$	$8i$
(200)			$6f; 6g$	$12j$	$12k$	$2\times 12j$	$2\times 12k$	$24l$	$2\times 24l$
[4] $R\bar{3}m$	(rhombohedral axes)		$1a$	$1b$	$3e$	$3d$	$6h$	$6h$	$2c; 6h$
(166)			$12i$	$6f; 6h$	$6g; 6h$	$2\times 12i$	$2\times 12i$	$2\times 6h; 12i$	$4\times 12i$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$,	$\frac{1}{3}(2x-y-z), \frac{1}{3}(x+y-2z)$,	$3a$	$3b$	$9e$	$9d$	$18h$	$18h$	$6c; 18h$
	$\mathbf{a}+\mathbf{b}+\mathbf{c}$	$\frac{1}{3}(x+y+z)$	$36i$	$18f; 18h$	$18g; 18h$	$2\times 36i$	$2\times 36i$	$2\times 18h; 36i$	$4\times 36i$
	(hexagonal axes)								
conjugate:	$-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$,	$\frac{1}{3}(-2x-y+z), \frac{1}{3}(-x+y+2z)$,							
	$-\mathbf{a}+\mathbf{b}-\mathbf{c}$	$\frac{1}{3}(-x+y-z)$							
	(hexagonal axes)								
conjugate:	$\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$,	$\frac{1}{3}(2x+y+z), \frac{1}{3}(x-y+2z)$,							
	$\mathbf{a}-\mathbf{b}-\mathbf{c}$	$\frac{1}{3}(x-y-z)$							
	(hexagonal axes)								
conjugate:	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$,	$\frac{1}{3}(-2x+y-z), \frac{1}{3}(-x-y-2z)$,							
	$-\mathbf{a}-\mathbf{b}+\mathbf{c}$	$\frac{1}{3}(-x-y+z)$							
	(hexagonal axes)								
[3] $P4/mmm$			$1a$	$1d$	$1c; 2e$	$1b; 2f$	$2g; 4l$	$2h; 4o$	$8r$
(123)			$4i; 4m; 4n$	$4j; 8s$	$4k; 8t$	$8p; 2\times 8s$	$8q; 2\times 8t$	$8r; 16u$	$3\times 16u$
conjugate:	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x							
conjugate:	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y							

II Maximal *klassengleiche* subgroups

Enlarged unit cell, non-isomorphic

[2] $Fm\bar{3}c$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z; +(\frac{1}{2},0,0)$	$8b$	$8a$	$24d$	$24c$	$48e$	$48f$	$64g$
(226)			$96i$	$96i$	$96h$	$2\times 96i$	$192j$	$192j$	$2\times 192j$
[2] $Fm\bar{3}c$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$;	$8a$	$8b$	$24c$	$24d$	$48f$	$48e$	$64g$
(226)		$+(\frac{1}{2},0,0)$	$96i$	$96h$	$96i$	$192j$	$2\times 96i$	$192j$	$2\times 192j$
[2] $Fm\bar{3}m$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z; +(\frac{1}{2},0,0)$	$4a; 4b$	$8c$	$24d$	$24e$	$2\times 24e$	$48g$	$2\times 32f$
(225)			$96j$	$24h; 48i$	$96k$	$2\times 96j$	$192l$	$2\times 96k$	$2\times 192l$
[2] $Fm\bar{3}m$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$;	$8c$	$4a; 4b$	$24e$	$24d$	$48g$	$2\times 24e$	$2\times 32f$
(225)		$+(\frac{1}{2},0,0)$	$96j$	$96k$	$48h; 48i$	$192l$	$2\times 96j$	$2\times 96k$	$2\times 192l$
[4] $Im\bar{3}m$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z; +(\frac{1}{2},0,0)$;	$2a; 6b$	$8c$	$24h$	$12d; 12e$	$2\times 12e; 24g$	$48k$	$16f; 48k$
(229)		$+(0,\frac{1}{2},0); +(0,0,\frac{1}{2})$	$2\times 48j$	$2\times 24h; 48j$	$48i; 48k$	$4\times 48j$	$2\times 96l$	$2\times 48k; 96l$	$4\times 96l$
[4] $Im\bar{3}m$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$;	$8c$	$2a; 6b$	$12d; 12e$	$24h$	$48k$	$2\times 12e; 24g$	$16f; 48k$
(229)		$(\frac{1}{2},0,0); +(0,\frac{1}{2},0)$;	$2\times 48j$	$48i; 48k$	$2\times 24h; 48j$	$2\times 96l$	$4\times 48j$	$2\times 48k; 96l$	$4\times 96l$
		$+(0,0,\frac{1}{2})$							

Axes	Coordinates	Wyckoff positions $1a$	$1b$ $8g$	$3c$ $12h$	$3d$ $12i$ $24l$	$6e$ $12j$ $24m$	$6f$ $24k$ $48n$
Enlarged unit cell, isomorphic							
[27] $Pm\bar{3}m$ $3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$1a; 6e; 8g; 12i$	$1b; 6f; 8g; 12j$	$3c; 6f; 12h; 12i; 24l; 24m$	$3d; 6e; 12h; 12j; 24k; 24m$	$3\times 6e; 3\times 24k; 3\times 24m$	$3\times 6f; 3\times 24l; 3\times 24m$
			$3\times 8g; 6\times 24m; 48n$	$3\times 12h; 3\times 24k; 3\times 24l; 3\times 48n$	$3\times 12i; 3\times 24k; 3\times 24m; 3\times 48n$	$3\times 12j; 3\times 24l; 3\times 24m; 3\times 48n$	$9\times 24k; 9\times 48n$
					$9\times 24l; 9\times 48n$	$9\times 24m; 9\times 48n$	$27\times 48n$
$[p^3]$ $Pm\bar{3}m$ $p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$ $u,v,w = 1,\ldots,p-1$	$1a; \frac{p-1}{2}\times 6e$; $\frac{p-1}{2}\times 8g$; $\frac{p-1}{2}\times 12i$; $\frac{(p-1)(p-3)}{8}\times 24k$; $\frac{(p-1)(p-3)}{4}\times 24m$; $\frac{(p-1)(p-3)(p-5)}{48}\times 48n$	$1b; \frac{p-1}{2}\times 6f$; $\frac{p-1}{2}\times 8g$; $\frac{p-1}{2}\times 12j$; $\frac{(p-1)(p-3)}{8}\times 24l$; $\frac{(p-1)(p-3)}{4}\times 24m$; $\frac{(p-1)(p-3)(p-5)}{48}\times 48n$	$3c; \frac{p-1}{2}\times 6f$; $\frac{p-1}{2}\times 12h$; $\frac{p-1}{2}\times 12i$; $\frac{(p-1)(p-3)}{8}\times 24k$; $\frac{(p-1)^2}{4}\times 24l$; $\frac{(p-1)^2}{4}\times 24m$; $\frac{(p-1)^2(p-3)}{16}\times 48n$	$3d; \frac{p-1}{2}\times 6e$; $\frac{p-1}{2}\times 12h$; $\frac{p-1}{2}\times 12j$; $\frac{(p-1)^2}{4}\times 24k$; $\frac{(p-1)(p-3)}{8}\times 24l$; $\frac{(p-1)^2}{4}\times 24m$; $\frac{(p-1)^2(p-3)}{16}\times 48n$	$p\times 6e$; $\frac{p(p-1)}{2}\times 24k$; $\frac{p(p-1)}{2}\times 24m$; $\frac{p(p-1)(p-3)}{8}\times 48n$	$p\times 6f$; $\frac{p(p-1)}{2}\times 24l$; $\frac{p(p-1)}{2}\times 24m$; $\frac{p(p-1)(p-3)}{8}\times 48n$
			$p\times 8g$; $p(p-1)\times 24m$; $\frac{p(p-1)(p-2)}{6}\times 48n$	$p\times 12h$; $\frac{p(p-1)}{2}\times 24k$; $\frac{p(p-1)}{2}\times 24l$; $\frac{p(p-1)^2}{4}\times 48n$	$p\times 12i$; $\frac{p(p-1)}{2}\times 24k$; $\frac{p(p-1)}{2}\times 24m$; $\frac{p(p-1)^2}{4}\times 48n$	$p\times 12j$; $\frac{p(p-1)}{2}\times 24l$; $\frac{p(p-1)}{2}\times 24m$; $\frac{p(p-1)^2}{4}\times 48n$	$p^2\times 24k$; $\frac{p^2(p-1)}{2}\times 48n$
					$p^2\times 24l$; $\frac{p^2(p-1)}{2}\times 48n$	$p^2\times 24m$; $\frac{p^2(p-1)}{2}\times 48n$	$p^3\times 48n$

$Pn\bar{3}n$ No. 222 $P4/n\bar{3}2/n$ O_h^2

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions 2a	6b	8c	12d 24g	12e 24h	16f 48i
I Maximal *translationengleiche* subgroups									
[2] $P\bar{4}3n$ (218)			$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	2a	6b	8e	6c; 6d 12g; 12h	12f 24i	2×8e 2×24i
[2] $P432$ (207)			$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	1a; 1b	3c; 3d	8g	12h 2×12h	6e; 6f 12i; 12j	2×8g 2×24k
[2] $Pn\bar{3}$ (201)				2a	6d	4b; 4c	12g 2×12g	12f 24h	2×8e 2×24h
[4] $R\bar{3}c$ (167) (rhombohedral axes)		$x-\frac{1}{4},y-\frac{1}{4},z-\frac{1}{4}$		2a	6e	2b; 6d	12f 2×12f	12f 2×6e; 12f	4c; 12f 4×12f
	a−**b**, **b**−**c**, **a**+**b**+**c** (hex. axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)-\frac{1}{4}$	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	6a	18e	6b; 18d	36f 2×36f	36f 2×18e; 36f	12c; 36f 4×36f
conjugate:	−**a**−**b**, **b**+**c**, −**a**+**b**−**c** (hex. axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)-\frac{1}{4}$	$\frac{1}{3}(-2x-y+z)+\frac{1}{2}$, $\frac{1}{3}(-x+y+2z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-z)$						
conjugate:	**a**+**b**, −**b**+**c**, **a**−**b**−**c** (hex. axes)	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)-\frac{1}{4}$	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)+\frac{1}{2}$, $\frac{1}{3}(x-y-z)$						
conjugate:	−**a**+**b**, −**b**−**c**, −**a**−**b**+**c** (hex. axes)	$\frac{1}{3}(-2x+y-z)$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)-\frac{1}{4}$	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$						
[3] $P4/nnc$ (126)				2a	2b; 4c	8f	4d; 8j 8g; 2×8j	4e; 8i 8h; 16k	16k 3×16k
conjugate:	**b**, **c**, **a**	y,z,x	y,z,x						
conjugate:	**c**, **a**, **b**	z,x,y	z,x,y						

II Maximal *klassengleiche* subgroups
Enlarged unit cell, isomorphic

	Axes	Coordinates origin 1	Coordinates origin 2	2a	6b	8c	12d 24g	12e 24h	16f 48i
[27] $Pn\bar{3}n$	3**a**, 3**b**, 3**c**	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z$;	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z$;	2a; 12e; 16f; 24h	6b; 12e; 24g; 24h; 2×48i	8c; 16f; 4×48i	12d; 24g; 6×48i 3×24g; 12×48i	3×12e; 6×48i 3×24h; 12×48i	3×16f; 8×48i 27×48i
		$\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$							
[p^3] $Pn\bar{3}n$	p**a**, p**b**, p**c**	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	$\frac{1}{p}x,\frac{1}{p}y,\frac{1}{p}z$; $+(\frac{u}{p},\frac{v}{p},\frac{w}{p})$	2a; $\frac{p-1}{2}$×12e; $\frac{p-1}{2}$×16f; $\frac{p-1}{2}$×24h; $\frac{p^3-13p+12}{24}$×48i	6b; $\frac{p-1}{2}$×12e; $\frac{p-1}{2}$×24g; $\frac{p-1}{2}$×24h; $\frac{p^3-5p+4}{8}$×48i	8c; $\frac{p-1}{2}$×16f; $\frac{p(p^2-1)}{6}$×48i	12d; $\frac{p-1}{2}$×24g; $\frac{p(p^2-1)}{4}$×48i p×24g; $\frac{p(p^2-1)}{2}$×48i	p×12e; $\frac{p(p^2-1)}{4}$×48i p×24h; $\frac{p(p^2-1)}{2}$×48i	p×16f; $\frac{p(p^2-1)}{3}$×48i p^3×48i
	p = prime > 2; $u,v,w = 1,\ldots,p-1$								

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 223, pp. 711–712.

O_h^3 $P4_2/m\bar{3}2/n$ No. 223 $Pm\bar{3}n$

	Axes	Coordinates	Wyckoff positions						
			$2a$	$6b$	$6c$ $12h$	$6d$ $16i$	$8e$ $24j$	$12f$ $24k$	$12g$ $48l$
I Maximal *translationengleiche* subgroups									
[2] $P\bar{4}3n$ (218)			$2a$	$6b$	$6d$ $12g$	$6c$ $2{\times}8e$	$8e$ $24i$	$12f$ $24i$	$12h$ $2{\times}24i$
[2] $P4_232$ (208)			$2a$	$6d$	$6e$ $12j$	$6f$ $2{\times}8g$	$4b;4c$ $12k;12l$	$12h$ $24m$	$12i$ $2{\times}24m$
[2] $Pm\bar{3}$ (200)			$1a;1b$	$3c;3d$	$6f$ $2{\times}6g$	$6g$ $2{\times}8i$	$8i$ $24l$	$6e;6h$ $12j;12k$	$2{\times}6f$ $2{\times}24l$
[4] $R\bar{3}c$ (167)	(rhombohedral axes)		$2b$	$6d$	$6e$ $12f$	$6e$ $4c;12f$	$2a;6e$ $2{\times}6e;12f$	$12f$ $2{\times}12f$	$12f$ $4{\times}12f$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x-y-z), \frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$6b$	$18d$	$18e$ $36f$	$18e$ $12c;36f$	$6a;18e$ $2{\times}18e;36f$	$36f$ $2{\times}36f$	$36f$ $4{\times}36f$
conjugate:	$-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x-y+z), \frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)$							
conjugate:	$\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(2x+y+z), \frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)$							
conjugate:	$-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{1}{3}(-2x+y-z), \frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$							
[3] $P4_2/mmc$ (131)		$x+\frac{1}{2},y,z$	$2d$	$2a;2b;2c$	$2f;4l$ $4g;2{\times}4m$	$2e;4m$ $16r$	$8n$ $8n;16r$	$4i;4j;4k$ $8o;8p;8q$	$4h;2{\times}4l$ $3{\times}16r$
conjugate:	$\mathbf{b},\mathbf{c},\mathbf{a}$	$y+\frac{1}{2},z,x$							
conjugate:	$\mathbf{c},\mathbf{a},\mathbf{b}$	$z+\frac{1}{2},x,y$							
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[4] $Ia\bar{3}d$ (230)	$2\mathbf{a}$, $2\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}x,\frac{1}{2}y,\frac{1}{2}z;+(\frac{1}{2},0,0)$; $+(0,\frac{1}{2},0);+(0,0,\frac{1}{2})$	$16a$	$48f$	$24c;24d$ $96h$	$48g$ $32e;96h$	$16b;48g$ $2{\times}48g;96h$	$96h$ $2{\times}96h$	$2{\times}48f$ $4{\times}96h$
[4] $Ia\bar{3}d$ (230)	$2\mathbf{a}$, $2\mathbf{b}$, $2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4},\frac{1}{2}y+\frac{1}{4},\frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0);+(0,\frac{1}{2},0)$; $+(0,0,\frac{1}{2})$	$16a$	$48f$	$48g$ $2{\times}48f$	$24c;24d$ $32e;96h$	$16b;48g$ $2{\times}48g;96h$	$96h$ $2{\times}96h$	$96h$ $4{\times}96h$
Enlarged unit cell, isomorphic									
[27] $Pm\bar{3}n$	$3\mathbf{a}$, $3\mathbf{b}$, $3\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z;\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0);\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0);\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$2a;12f$; $16i;24k$	$6b;12f$; $12g;12h$; $3{\times}24k;48l$	$6c;12g$; $24j$; $3{\times}24k;48l$ $3{\times}12h$; $6{\times}24k$; $3{\times}48l$	$6d;12h$; $24j$; $3{\times}24k;48l$ $3{\times}16i$; $8{\times}48l$	$8e;16i$; $2{\times}24j$; $3{\times}48l$ $3{\times}24j$; $12{\times}48l$	$3{\times}12f$; $6{\times}24k$; $3{\times}48l$ $9{\times}24k$; $9{\times}48l$	$3{\times}12g$; $6{\times}24k$; $3{\times}48l$ $27{\times}48l$

Axes	Coordinates	2a / 12g	6b / 12h	6c / 16i	6d / 24j	8e / 24k	12f / 48l
$[p^3]$ $Pm\bar{3}n$ $p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$; p = prime > 2; $u,v,w = 1,\ldots,p-1$	$2a$; $\frac{p-1}{2}\times 12f$; $\frac{p-1}{2}\times 16i$; $\frac{(p-1)^2}{4}\times 24k$; $\frac{(p^2-1)(p-3)}{24}\times 48l$	$6b$; $\frac{p-1}{2}\times 12f$; $\frac{p-1}{2}\times 12g$; $\frac{p-1}{2}\times 12h$; $\frac{3(p-1)^2}{4}\times 24k$; $\frac{(p-1)^3}{8}\times 48l$	$6c$; $\frac{p-1}{2}\times 12g$; $\frac{p-1}{2}\times 24j$; $\frac{p(p-1)}{2}\times 24k$; $\frac{(p^2-1)(p-2)}{8}\times 48l$	$6d$; $\frac{p-1}{2}\times 12h$; $\frac{p-1}{2}\times 24j$; $\frac{p(p-1)}{2}\times 24k$; $\frac{(p^2-1)(p-2)}{8}\times 48l$	$8e$; $\frac{p-1}{2}\times 16i$; $(p-1)\times 24j$; $\frac{p^3-4p+3}{6}\times 48l$	$p\times 12f$; $p(p-1)\times 24k$; $\frac{p(p-1)^2}{4}\times 48l$
		$p\times 12g$; $p(p-1)\times 24k$; $\frac{p(p-1)^2}{4}\times 48l$	$p\times 12h$; $p(p-1)\times 24k$; $\frac{p(p-1)^2}{4}\times 48l$	$p\times 16i$; $\frac{p(p^2-1)}{3}\times 48l$	$p\times 24j$; $\frac{p(p^2-1)}{2}\times 48l$	$p^2\times 24k$; $\frac{p^2(p-1)}{2}\times 48l$	$p^3\times 48l$

$Pn\bar{3}m$ No. 224 $P4_2/n\bar{3}2/m$ CONTINUED (*from next page*)

Axes	Coordinates origin 1	Coordinates origin 2	2a	4b / 12f	4c / 12g / 24j	6d / 24h / 24k	8e / 24i / 48l
Enlarged unit cell, isomorphic							
[27] $Pn\bar{3}m$ $3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$;	$2a$; $2\times 8e$; $12g$; $24k$	$4b(c^*)$; $8e$; $24i(j^*)$; $3\times 24k$	$4c(b^*)$; $8e$; $24j(i^*)$; $3\times 24k$	$6d$; $12g$; $24h$; $3\times 24k$; $48l$	$3\times 8e$; $6\times 24k$; $48l$
	$\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$			$12f$; $24h$; $24i$; $24j$; $5\times 48l$	$3\times 12g$; $6\times 24k$; $3\times 48l$	$3\times 24h$; $12\times 48l$	$3\times 24i(j^*)$; $12\times 48l$
					$3\times 24j(i^*)$; $12\times 48l$	$9\times 24k$; $9\times 48l$	$27\times 48l$
$[p^3]$ $Pn\bar{3}m$ $p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$; p = prime > 2;	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$ $u,v,w = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$2a$; $(p-1)\times 8e$; $\frac{p-1}{2}\times 12g$; $\frac{(p-1)(p-2)}{2}\times 24k$; $\frac{(p-1)(p-2)(p-3)}{24}\times 48l$	$4b(c^\dagger)$; $\frac{p-1}{2}\times 8e$; $\frac{p-1}{2}\times 24i(j^\dagger)$; $\frac{p(p-1)}{2}\times 24k$; $\frac{(p^2-1)(p-3)}{12}\times 48l$	$4c(b^\dagger)$; $\frac{p-1}{2}\times 8e$; $\frac{p-1}{2}\times 24j(i^\dagger)$; $\frac{p(p-1)}{2}\times 24k$; $\frac{(p^2-1)(p-3)}{12}\times 48l$	$6d$; $\frac{p-1}{2}\times 12g$; $\frac{p-1}{2}\times 24h$; $\frac{p(p-1)}{2}\times 24k$; $\frac{(p^2-1)(p-2)}{8}\times 48l$	$p\times 8e$; $p(p-1)\times 24k$; $\frac{p(p-1)(p-2)}{6}\times 48l$
				$12f$; $\frac{p-1}{2}\times 24h$; $\frac{p-1}{2}\times 24i$; $\frac{p-1}{2}\times 24j$; $\frac{(p-1)^2(p+2)}{4}\times 48l$	$p\times 12g$; $p(p-1)\times 24k$; $\frac{p(p-1)^2}{4}\times 48l$	$p\times 24h$; $\frac{p(p^2-1)}{2}\times 48l$	$p\times 24i(j^\dagger)$; $\frac{p(p^2-1)}{2}\times 48l$
					$p\times 24j(i^\dagger)$; $\frac{p(p^2-1)}{2}\times 48l$	$p^2\times 24k$; $\frac{p^2(p-1)}{2}\times 48l$	$p^3\times 48l$

* origin 1

† origin 1 and $p = 4n-1$

O_h^4 $P4_2/n\bar{3}2/m$ No. 224 $Pn\bar{3}m$

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions					
				$2a$	$4b$	$4c$	$6d$	$8e$	$12f$
				$12g$	$24h$	$24i$	$24j$	$24k$	$48l$
I Maximal *translationengleiche* subgroups									
[2] $P\bar{4}3m$			$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$1a; 1b$	$4e$	$4e$	$3c; 3d$	$2\times4e$	$12h$
(215)				$6f; 6g$	$2\times12h$	$24j$	$24j$	$2\times12i$	$2\times24j$
[2] $P4_232$			$x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	$2a$	$4b$	$4c$	$6d$	$8g$	$6e; 6f$
(208)				$12h$	$12i; 12j$	$2\times12k$	$2\times12l$	$24m$	$2\times24m$
[2] $Pn\bar{3}$				$2a$	$4b$	$4c$	$6d$	$8e$	$12g$
(201)				$12f$	$2\times12g$	$24h$	$24h$	$24h$	$2\times24h$
[4] $R\bar{3}m$		$x-\frac{1}{4}, y-\frac{1}{4}, z-\frac{1}{4}$		$2c$	$1a; 3e$	$1b; 3d$	$6h$	$2c; 6h$	$6f; 6g$
(166)	(rhombohedral axes)			$2\times6h$	$2\times12i$	$2\times6f; 12i$	$2\times6g; 12i$	$2\times6h; 12i$	$4\times12i$
	$\mathbf{a}-\mathbf{b}$, $\mathbf{b}-\mathbf{c}$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)-\frac{1}{4}$	$\frac{1}{3}(2x-y-z)$, $\frac{1}{3}(x+y-2z)$, $\frac{1}{3}(x+y+z)$	$6c$	$3a; 9e$	$3b; 9d$	$18h$	$6c; 18h$	$18f; 18g$
				$2\times18h$	$2\times36i$	$2\times18f; 36i$	$2\times18g; 36i$	$2\times18h; 36i$	$4\times36i$
	conjugate: $-\mathbf{a}-\mathbf{b}$, $\mathbf{b}+\mathbf{c}$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x-y+z)$, $\frac{1}{3}(-x+y+2z)$, $\frac{1}{3}(-x+y-z)-\frac{1}{4}$	$\frac{1}{3}(-2x-y+z)+\frac{1}{2}$, $\frac{1}{3}(-x+y+2z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-z)$						
	conjugate: $\mathbf{a}+\mathbf{b}$, $-\mathbf{b}+\mathbf{c}$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hex. axes)	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)$, $\frac{1}{3}(x-y-z)-\frac{1}{4}$	$\frac{1}{3}(2x+y+z)$, $\frac{1}{3}(x-y+2z)+\frac{1}{2}$, $\frac{1}{3}(x-y-z)$						
	conjugate: $-\mathbf{a}+\mathbf{b}$, $-\mathbf{b}-\mathbf{c}$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hex. axes)	$\frac{1}{3}(-2x+y-z)$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)-\frac{1}{4}$	$\frac{1}{3}(-2x+y-z)+\frac{1}{2}$, $\frac{1}{3}(-x-y-2z)$, $\frac{1}{3}(-x-y+z)$						
[3] $P4_2/nnm$			$x, y+\frac{1}{2}, z$	$2a$	$4e$	$4f$	$2b; 4c$	$8m$	$4d; 8j$
(134)				$4g; 8i$	$8h; 2\times8j$	$8l; 16n$	$8k; 16n$	$8m; 16n$	$3\times16n$
	conjugate: $\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x	$y+\frac{1}{2}, z, x$						
	conjugate: $\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y	$z, x, y+\frac{1}{2}$						
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, non-isomorphic									
[2] $Fd\bar{3}c$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$16a$	$32c$	$32b$	$48d$	$64e$	$96g$
(228)				$96f$	$192h$	$192h$	$2\times96g$	$192h$	$2\times192h$
[2] $Fd\bar{3}c$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$16a$	$32b$	$32c$	$48d$	$64e$	$96g$
(228)				$96f$	$192h$	$2\times96g$	$192h$	$192h$	$2\times192h$
[2] $Fd\bar{3}m$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$; $+(\frac{1}{2},0,0)$	$8a; 8b$	$16c; 16d$	$32e$	$48f$	$2\times32e$	$96h$
(227)				$2\times48f$	$192i$	$2\times96h$	$192i$	$2\times96g$	$2\times192i$
[2] $Fd\bar{3}m$	$2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$\frac{1}{2}x+\frac{1}{4}, \frac{1}{2}y+\frac{1}{4}, \frac{1}{2}z+\frac{1}{4}$; $+(\frac{1}{2},0,0)$	$8a; 8b$	$32e$	$16c; 16d$	$48f$	$2\times32e$	$96h$
(227)				$2\times48f$	$192i$	$192i$	$2\times96h$	$2\times96g$	$2\times192i$

Continued on preceding page

International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 225, pp. 714–715.

$Fm\bar{3}m$ No. 225 $F4/m\bar{3}2/m$ O_h^5

	Axes	Coordinates	Wyckoff positions						
			$4a$	$4b$	$8c$ $48h$	$24d$ $48i$	$24e$ $96j$	$32f$ $96k$	$48g$ $192l$

I Maximal *translationengleiche* subgroups

	Axes	Coordinates	$4a$	$4b$	$8c$ / $48h$	$24d$ / $48i$	$24e$ / $96j$	$32f$ / $96k$	$48g$ / $192l$
[2] $F\bar{4}3m$ (216)			$4a$	$4b$	$4c; 4d$ $48h$	$24g$ $48h$	$24f$ $96i$	$2\times16e$ $2\times48h$	$2\times24g$ $2\times96i$
[2] $F432$ (209)			$4a$	$4b$	$8c$ $48g$	$24d$ $48h$	$24e$ $96j$	$32f$ $96j$	$48i$ $2\times96j$
[2] $Fm\bar{3}$ (202)			$4a$	$4b$	$8c$ $48h$	$24d$ $48h$	$24e$ $2\times48h$	$32f$ $96i$	$48g$ $2\times96i$
[4] $R\bar{3}m$ (166)	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhomboh. axes)	$-x+y+z$, $x-y+z$, $x+y-z$	$1a$	$1b$	$2c$ $6f; 6h$	$3d; 3e$ $6g; 6h$	$6h$ $2\times12i$	$2c; 6h$ $2\times6h; 12i$	$2\times6h$ $4\times12i$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(-\mathbf{b}+\mathbf{c})$, $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z)$, $\frac{2}{3}(-x-y+2z)$, $\frac{1}{3}(x+y+z)$	$3a$	$3b$	$6c$ $18f; 18h$	$9d; 9e$ $18g; 18h$	$18h$ $2\times36i$	$6c; 18h$ $2\times18h; 36i$	$2\times18h$ $4\times36i$
conjugate:	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(-\mathbf{b}-\mathbf{c})$, $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z)$, $\frac{2}{3}(x-y-2z)$, $\frac{1}{3}(-x+y-z)$							
conjugate:	$\frac{1}{2}(-\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{b}-\mathbf{c})$, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z)$, $\frac{2}{3}(-x+y-2z)$, $\frac{1}{3}(x-y-z)$							
conjugate:	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z)$, $\frac{2}{3}(x+y+2z)$, $\frac{1}{3}(-x-y+z)$							
[3] $I4/mmm$ (139)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\mathbf{c}$	$x-y, x+y, z$	$2a$	$2b$	$4d$ $8i; 16m$	$4c; 8f$ $8j; 16m$	$4e; 8h$ $16l; 2\times16m$	$16n$ $16n; 32o$	$8g; 16k$ $3\times32o$
conjugate:	$\frac{1}{2}(\mathbf{b}-\mathbf{c})$, $\frac{1}{2}(\mathbf{b}+\mathbf{c})$, $\mathbf{a}$	$y-z, y+z, x$							
conjugate:	$\frac{1}{2}(-\mathbf{a}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\mathbf{b}$	$-x+z, x+z, y$							

II Maximal *klassengleiche* subgroups

Loss of centring translations

	Axes	Coordinates	$4a$	$4b$	$8c$ / $48h$	$24d$ / $48i$	$24e$ / $96j$	$32f$ / $96k$	$48g$ / $192l$
[4] $Pn\bar{3}m$ (224)	4 conjugate subgroups	origin 1: $x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$ origin 2: x, y, z	$4b$	$4c$	$2a; 6d$ $24i; 24k$	$12f; 12g$ $24j; 24k$	$24k$ $2\times48l$	$8e; 24k$ $2\times24k; 48l$	$2\times12g; 24h$ $4\times48l$
[4] $Pm\bar{3}m$ (221)	4 conjugate subgroups		$1a; 3c$	$1b; 3d$	$8g$ $2\times12i; 24l$	$12i; 12j$ $2\times12j; 24k$	$6e; 6f; 12h$ $2\times24k; 2\times24l$	$8g; 24m$ $2\times24m; 48n$	$2\times24m$ $4\times48n$

Enlarged unit cell, isomorphic

	Axes	Coordinates	$4a$	$4b$	$8c$ / $48h$	$24d$ / $48i$	$24e$ / $96j$	$32f$ / $96k$	$48g$ / $192l$
[27] $Fm\bar{3}m$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$4a; 24e$; $32f; 48h$	$4b; 24e$; $32f; 48i$	$8c; 2\times32f$; $48g; 96k$ $3\times48h$; $3\times96j$; $3\times96k$; $3\times192l$	$24d; 48g$; $48h; 48i$; $96j; 2\times96k$; $192l$ $3\times48i$; $3\times96j$; $3\times96k$; $3\times192l$	$3\times24e$; $3\times96j$; $3\times96k$ $9\times96j$; $9\times192l$	$3\times32f$; $6\times96k$; $192l$ $9\times96k$; $9\times192l$	$3\times48g$; $6\times96k$; $3\times192l$ $27\times192l$

Axes	Coordinates	Wyckoff positions 4a 48g	 4b 48h	 8c 48i	 24d 96j	 24e 96k	 32f 192l
$[p^3]\,Fm\bar{3}m$ $p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2; $u,v,w = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$4a; \frac{p-1}{2}\times 24e$; $\frac{p-1}{2}\times 32f$; $\frac{p-1}{2}\times 48h$; $\frac{(p-1)(p-3)}{8}\times 96j$; $\frac{(p-1)(p-3)}{4}\times 96k$; $\frac{(p-1)(p-3)(p-5)}{48}\times 192l$	$4b; \frac{p-1}{2}\times 24e$; $\frac{p-1}{2}\times 32f$; $\frac{p-1}{2}\times 48i$; $\frac{(p-1)(p-3)}{8}\times 96j$; $\frac{(p-1)(p-3)}{4}\times 96k$; $\frac{(p-1)(p-3)(p-5)}{48}\times 192l$	$8c; (p-1)\times 32f$; $\frac{p-1}{2}\times 48g$; $\frac{(p-1)(p-2)}{2}\times 96k$; $\frac{(p-1)(p-2)(p-3)}{24}\times 192l$	$24d; \frac{p-1}{2}\times 48g$; $\frac{p-1}{2}\times 48h$; $\frac{p-1}{2}\times 48i$; $\frac{(p-1)^2}{4}\times 96j$; $\frac{(p-1)^2}{2}\times 96k$; $\frac{(p-1)^3}{8}\times 192l$	$p\times 24e$; $\frac{p(p-1)}{2}\times 96j$; $\frac{p(p-1)}{2}\times 96k$; $\frac{p(p-1)(p-3)}{8}\times 192l$	$p\times 32f$; $p(p-1)\times 96k$; $\frac{p(p-1)(p-2)}{6}\times 192l$
		$p\times 48g$; $p(p-1)\times 96k$; $\frac{p(p-1)^2}{4}\times 192l$	$p\times 48h$; $\frac{p(p-1)}{2}\times 96j$; $\frac{p(p-1)}{2}\times 96k$; $\frac{p(p-1)^2}{4}\times 192l$	$p\times 48i$; $\frac{p(p-1)}{2}\times 96j$; $\frac{p(p-1)}{2}\times 96k$; $\frac{p(p-1)^2}{4}\times 192l$	$p^2\times 96j$; $\frac{p^2(p-1)}{2}\times 192l$	$p^2\times 96k$; $\frac{p^2(p-1)}{2}\times 192l$	$p^3\times 192l$

Axes	Coordinates	Wyckoff positions 8a	 8b	 24c 64g	 24d 96h	 48e 96i	 48f 192j
$[p^3]\,Fm\bar{3}c$ $p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2; $u,v,w = 1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$8a; \frac{p-1}{2}\times 48f$; $\frac{p-1}{2}\times 64g$; $\frac{p-1}{2}\times 96h$; $\frac{(p-1)(p-3)(p+4)}{24}\times 192j$	$8b; \frac{p-1}{2}\times 48e$; $\frac{p-1}{2}\times 64g$; $\frac{(p-1)^2}{4}\times 96i$; $\frac{(p^2-1)(p-3)}{24}\times 192j$	$24c; \frac{p-1}{2}\times 48e$; $\frac{p-1}{2}\times 96h$; $\frac{p(p-1)}{2}\times 96i$; $\frac{(p^2-1)(p-2)}{8}\times 192j$	$24d; \frac{p-1}{2}\times 48f$; $\frac{p^2-1}{4}\times 96i$; $\frac{(p-1)(p^2-1)}{8}\times 192j$	$p\times 48e$; $p(p-1)\times 96i$; $\frac{p(p-1)^2}{4}\times 192j$	$p\times 48f$; $\frac{p(p^2-1)}{4}\times 192j$
				$p\times 64g$; $\frac{p(p^2-1)}{3}\times 192j$	$p\times 96h$; $\frac{p(p^2-1)}{2}\times 192j$	$p^2\times 96i$; $\frac{p^2(p-1)}{2}\times 192j$	$p^3\times 192j$

$Fm\bar{3}c$ No. 226 $F\,4/m\,\bar{3}\,2/c$ O_h^6

	Axes	Coordinates	Wyckoff positions						
			$8a$	$8b$	$24c$	$24d$	$48e$ $96h$	$48f$ $96i$	$64g$ $192j$
I Maximal *translationengleiche* subgroups									
[2] $F\bar{4}3c$ (219)			$8b$	$8a$	$24d$	$24c$	$48f$ $96h$	$48g$ $96h$	$2\times32e$ $2\times96h$
[2] $F432$ (209)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	$4a;4b$	$8c$	$24d$	$24e$	$48i$ $48g;48h$	$2\times24e$ $96j$	$2\times32f$ $2\times96j$
[2] $Fm\bar{3}$ (202)			$8c$	$4a;4b$	$24e$	$24d$	$2\times24e$ $96i$	$48g$ $2\times48h$	$2\times32f$ $2\times96i$
[4] $R\bar{3}c$ (167)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c}),$ $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhomboh. axes)	$-x+y+z,$ $x-y+z,$ $x+y-z$	$2a$	$2b$	$6e$	$6d$	$12f$ $2\times6e;12f$	$12f$ $2\times12f$	$4c;12f$ $4\times12f$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}),\frac{1}{2}(-\mathbf{b}+\mathbf{c}),$ $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)$	$6a$	$6b$	$18e$	$18d$	$36f$ $2\times6e;12f$	$36f$ $2\times12f$	$12c;36f$ $4\times12f$
conjugate:	$\frac{1}{2}(\mathbf{a}+\mathbf{b}),\frac{1}{2}(-\mathbf{b}-\mathbf{c}),$ $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z),$ $\frac{2}{3}(x-y-2z),$ $\frac{1}{3}(-x+y-z)$							
conjugate:	$\frac{1}{2}(-\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{b}-\mathbf{c}),$ $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z),$ $\frac{1}{3}(x-y-z)$							
conjugate:	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{b}+\mathbf{c}),$ $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z),$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)$							
[3] $I4/mcm$ (140)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{a}+\mathbf{b}),\mathbf{c}$	$x-y+\frac{1}{2},x+y,z$	$4a$	$4d$	$4b;8h$	$4c;8e$	$8g;2\times8h$ $16j;32m$	$8f;16i$ $16k;2\times16l$	$32m$ $3\times32m$
conjugate:	$\frac{1}{2}(\mathbf{b}-\mathbf{c}),\frac{1}{2}(\mathbf{b}+\mathbf{c}),\mathbf{a}$	$y-z+\frac{1}{2}z,y+z,x$							
conjugate:	$\frac{1}{2}(-\mathbf{a}+\mathbf{c}),\frac{1}{2}(\mathbf{a}+\mathbf{c}),\mathbf{b}$	$-x+z+\frac{1}{2},x+z,y$							
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[4] $Pm\bar{3}n$ (223) 4 conjugate subgroups			$8e$	$2a;6b$	$6c;6d;12f$	$24k$	$2\times12f;12g;12h$ $2\times24j;48l$	$48l$ $4\times24k$	$16i;48l$ $4\times48l$
[4] $Pn\bar{3}n$ (222) 4 conju. subgr.		origin 1: $x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$ origin 2: x,y,z	$2a;6b$	$8c$	$24h$	$12d;12e$	$48i$ $2\times24h;48i$	$2\times12e;24g$ $2\times48i$	$16f;48i$ $4\times48i$
Enlarged unit cell, isomorphic									
[27] $Fm\bar{3}c$	$3\mathbf{a},3\mathbf{b},3\mathbf{c}$	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z;\pm(\frac{1}{3},0,0);$ $\pm(0,\frac{1}{3},0);\pm(0,0,\frac{1}{3});$ $\pm(0,\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},0,\frac{1}{3});$ $\pm(\frac{1}{3},\frac{1}{3},0);\pm(0,\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},0,\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3});$ $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	$8a;48f;$ $64g;$ $96h$	$8b;48e;$ $64g;$ $96i$	$24c;48e;$ $96h;3\times96i;$ $192j$	$24d;48f;$ $2\times96i;$ $2\times192j$	$3\times48e;6\times96i;$ $3\times192j$ $3\times96h;$ $12\times192j$	$3\times48f;$ $6\times192j$ $9\times96i;$ $9\times192j$	$3\times64g;$ $8\times192j$ $27\times192j$

Continued on preceding page

O_h^7 $\quad F\,4_1/d\,\bar{3}\,2/m$ $\quad$ No. 227 $\quad F\,d\,\bar{3}\,m$

	Axes	Coordinates origin 1	Coordinates origin 2	Wyckoff positions $8a$	$8b$	$16c$	$16d$ $96g$	$32e$ $96h$	$48f$ $192i$
I Maximal *translationengleiche* subgroups									
[2] $F\bar{4}3m$ (216)			$x+\frac{1}{8}, y+\frac{1}{8},$ $z+\frac{1}{8}$	$4a; 4d$	$4b; 4c$	$16e$	$16e$ $2\times48h$	$2\times16e$ $96i$	$24f; 24g$ $2\times96i$
[2] $F4_132$ (210)			$x+\frac{1}{8}, y+\frac{1}{8},$ $z+\frac{1}{8}$	$8a$	$8b$	$16c$	$16d$ $96h$	$32e$ $2\times48g$	$48f$ $2\times96h$
[2] $Fd\bar{3}$ (203)				$8a$	$8b$	$16c$	$16d$ $96g$	$32e$ $96g$	$48f$ $2\times96g$
[4] $R\bar{3}m$ (166)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c}),$ $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhomboh. axes)	$-x+y+z-\frac{1}{8},$ $x-y+z-\frac{1}{8},$ $x+y-z-\frac{1}{8}$	$-x+y+z,$ $x-y+z,$ $x+y-z$	$2c$	$2c$	$1a; 3d$	$1b; 3e$ $2\times6h; 12i$	$2c; 6h$ $6f; 6g; 12i$	$2\times6h$ $4\times12i$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}+\mathbf{c}),$ $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)-\frac{1}{8}$	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)$	$6c$	$6c$	$3a; 9d$	$3b; 9e$ $2\times18h; 36i$	$6c; 18h$ $18f; 18g; 36i$	$2\times18h$ $4\times36i$
	conjugate: $\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}(-\mathbf{b}-\mathbf{c}),$ $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z),$ $\frac{2}{3}(x-y-2z),$ $\frac{1}{3}(-x+y-z)-\frac{1}{8}$	$\frac{2}{3}(2x+y-z)+\frac{1}{2},$ $\frac{2}{3}(x-y-2z)+\frac{1}{2},$ $\frac{1}{3}(-x+y-z)+\frac{1}{2}$						
	conjugate: $\frac{1}{2}(-\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}-\mathbf{c}),$ $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z),$ $\frac{1}{3}(x-y-z)-\frac{1}{8}$	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z)+\frac{1}{2},$ $\frac{1}{3}(x-y-z)+\frac{1}{2}$						
	conjugate: $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{b}+\mathbf{c}),$ $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z),$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)-\frac{1}{8}$	$\frac{2}{3}(2x-y+z)+\frac{1}{2},$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)+\frac{1}{2}$						
[3] $I4_1/amd$ (141)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$	$x-y, x+y, z$	$x-y, x+y+\frac{1}{2}, z$	$4a$	$4b$	$8c$	$8d$ $16h; 32i$	$16h$ $16f; 32i$	$8e; 16g$ $3\times32i$
	conjugate: $\frac{1}{2}(\mathbf{b}-\mathbf{c}), \frac{1}{2}(\mathbf{b}+\mathbf{c}), \mathbf{a}$	$y-z, y+z, x$	$y-z, y+z+\frac{1}{2}, x$						
	conjugate: $\frac{1}{2}(-\mathbf{a}+\mathbf{c}), \frac{1}{2}(\mathbf{a}+\mathbf{c}), \mathbf{b}$	$-x+z, x+z, y$	$-x+z, x+z+\frac{1}{2}, y$						
II Maximal *klassengleiche* subgroups **Enlarged unit cell, isomorphic**									
[27] $Fd\bar{3}m$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\underbrace{\frac{1}{3}x-\frac{1}{4}, \frac{1}{3}y-\frac{1}{4}, \frac{1}{3}z-\frac{1}{4} \quad \frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z;}$ $\pm(\frac{1}{3},0,0); \pm(0,\frac{1}{3},0); \pm(0,0,\frac{1}{3});$ $\pm(0,\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},0,\frac{1}{3}); \pm(\frac{1}{3},\frac{1}{3},0);$ $\pm(0,\frac{1}{3},\frac{2}{3}); \pm(\frac{1}{3},0,\frac{2}{3}); \pm(\frac{1}{3},\frac{2}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{2}{3},\frac{1}{3},\frac{1}{3}); \pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});$ $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$		$8b;$ $2\times32e;$ $48f; 96g$	$8a;$ $2\times32e;$ $48f; 96g$	$16c; 32e;$ $3\times96g;$ $96h$	$16d; 32e;$ $3\times96g;$ $96h$ $9\times96g;$ $9\times192i$	$3\times32e;$ $6\times96g;$ $192i$ $3\times96h;$ $12\times192i$	$3\times48f;$ $6\times96g;$ $3\times192i$ $27\times192i$

Axes		Coordinates origin 1	Coordinates origin 2	Wyckoff positions: $8a$	$8b$ / $48f$	$16c$ / $96g$	$16d$ / $96h$	$32e$ / $192i$
$[p^3]\,Fd\bar{3}m$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	$\frac{1}{p}x+s, \frac{1}{p}y+s, \frac{1}{p}z+s;$ $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$ $s=0$ if $p=8n+1$; $s=-\frac{1}{4}$ if $p=8n+3$; $s=\frac{1}{2}$ if $p=8n+5$; $s=\frac{1}{4}$ if $p=8n+7$ $p=$ prime >2; $u,v,w=1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z;$ $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$8a(b^*)$; $(p-1)\times 32e$; $\frac{p-1}{2}\times 48f$; $\frac{(p-1)(p-2)}{2}\times 96g$; $\frac{(p-1)(p-2)(p-3)}{24}\times 192i$	$8b(a^*)$; $(p-1)\times 32e$; $\frac{p-1}{2}\times 48f$; $\frac{(p-1)(p-2)}{2}\times 96g$; $\frac{(p-1)(p-2)(p-3)}{24}\times 192i$ $p\times 48f$; $p(p-1)\times 96g$; $\frac{p(p-1)^2}{4}\times 192i$	$16c$; $\frac{p-1}{2}\times 32e$; $\frac{p(p-1)}{2}\times 96g$; $\frac{p-1}{2}\times 96h$; $\frac{(p^2-1)(p-3)}{12}\times 192i$ $p^2\times 96g$; $\frac{p^2(p-1)}{2}\times 192i$	$16d$; $\frac{p-1}{2}\times 32e$; $\frac{p(p-1)}{2}\times 96g$; $\frac{p-1}{2}\times 96h$; $\frac{(p^2-1)(p-3)}{12}\times 192i$ $p\times 96h$; $\frac{p(p^2-1)}{2}\times 192i$	$p\times 32e$; $p(p-1)\times 96g$; $\frac{p(p-1)(p-2)}{6}\times 192i$ $p^3\times 192i$

* $p=8n\pm 3$

$Fd\bar{3}c$ No. 228 $F4_1/d\bar{3}2/c$ CONTINUED (*from next page*)

Axes		Coordinates origin 1	Coordinates origin 2	Wyckoff positions: $16a$	$32b$	$32c$ / $96f$	$48d$ / $96g$	$64e$ / $192h$
$[p^3]\,Fd\bar{3}c$	$\mathbf{a}, p\mathbf{b}, p\mathbf{c}$	$\frac{1}{p}x+s, \frac{1}{p}y+s, \frac{1}{p}z+s;$ $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$ $s=0$ if $p=4n+1$; $s=\frac{1}{4}$ if $p=4n-1$ $p=$ prime >2; $u,v,w=1,\ldots,p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z;$ $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$16a$; $(p-1)\times 64e$; $\frac{p-1}{2}\times 96f$; $\frac{(p-1)(p-2)(p+3)}{12}\times 192h$	$32b$; $\frac{p-1}{2}\times 64e$; $(p-1)\times 96g$; $\frac{p^3-4p+3}{6}\times 192h$	$32c$; $\frac{p-1}{2}\times 64e$; $\frac{p(p^2-1)}{6}\times 192h$ $p\times 96f$; $\frac{p(p^2-1)}{2}\times 192h$	$48d$; $\frac{p-1}{2}\times 96f$; $\frac{p(p^2-1)}{4}\times 192h$ $p\times 96g$; $\frac{p(p^2-1)}{2}\times 192h$	$p\times 64e$; $\frac{p(p^2-1)}{3}\times 192h$ $p^3\times 192h$

O_h^8 $F\,4_1/d\,\bar{3}\,2/c$ No. 228 $F\,d\,\bar{3}\,c$

	Axes	Coordinates origin 1	Coordinates origin 2	16*a*	32*b*	32*c*	48*d*	64*e* / 96*g*	96*f* / 192*h*
I Maximal *translationengleiche* subgroups									
[2] $F\bar{4}3c$ (219)			$x+\frac{1}{8},y+\frac{1}{8},z+\frac{1}{8}$	$8a;8b$	$32e$	$32e$	$24c;24d$	$2\times32e$ $96h$	$48f;48g$ $2\times96h$
[2] $F4_132$ (210)			$x-\frac{1}{8},y-\frac{1}{8},z-\frac{1}{8}$	$8a;8b$	$16c;16d$	$32e$	$48f$	$2\times32e$ $2\times48g$	$2\times48f$ $2\times96h$
[2] $Fd\bar{3}$ (203)		$x+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$		$8a;8b$	$32e$	$16c;16d$	$48f$	$2\times32e$ $96g$	$2\times48f$ $2\times96g$
[4] $R\bar{3}c$ (167)	$\frac{1}{2}(\mathbf{b}+\mathbf{c}),\frac{1}{2}(\mathbf{a}+\mathbf{c}),$ $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ (rhombo. axes)	$-x+y+z+\frac{1}{8},$ $x-y+z+\frac{1}{8},$ $x+y-z+\frac{1}{8}$	$-x+y+z,$ $x-y+z,$ $x+y-z$	$4c$	$2a;6e$	$2b;6d$	$12f$	$4c;12f$ $2\times6e;12f$	$2\times12f$ $4\times12f$
	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}),\frac{1}{2}(-\mathbf{b}+\mathbf{c}),$ $\mathbf{a}+\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)+\frac{1}{8}$	$\frac{2}{3}(-2x+y+z),$ $\frac{2}{3}(-x-y+2z),$ $\frac{1}{3}(x+y+z)$	$12c$	$6a;18e$	$6b;18d$	$36f$	$12c;36f$ $2\times18e;36f$	$2\times36f$ $4\times36f$
	conjugate: $\frac{1}{2}(\mathbf{a}+\mathbf{b}),\frac{1}{2}(-\mathbf{b}-\mathbf{c}),$ $-\mathbf{a}+\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x+y-z),$ $\frac{2}{3}(x-y-2z),$ $\frac{1}{3}(-x+y-z)+\frac{1}{8}$	$\frac{2}{3}(2x+y-z)+\frac{1}{2},$ $\frac{2}{3}(x-y-2z)+\frac{1}{2},$ $\frac{1}{3}(-x+y-z)+\frac{1}{2}$						
	conjugate: $\frac{1}{2}(-\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{b}-\mathbf{c}),$ $\mathbf{a}-\mathbf{b}-\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z),$ $\frac{1}{3}(x-y-z)+\frac{1}{8}$	$\frac{2}{3}(-2x-y-z),$ $\frac{2}{3}(-x+y-2z)+\frac{1}{2},$ $\frac{1}{3}(x-y-z)+\frac{1}{2}$						
	conjugate: $\frac{1}{2}(\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{b}+\mathbf{c}),$ $-\mathbf{a}-\mathbf{b}+\mathbf{c}$ (hexagonal axes)	$\frac{2}{3}(2x-y+z),$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)+\frac{1}{8}$	$\frac{2}{3}(2x-y+z)+\frac{1}{2},$ $\frac{2}{3}(x+y+2z),$ $\frac{1}{3}(-x-y+z)+\frac{1}{2}$						
[3] $I4_1/acd$ (142)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{a}+\mathbf{b}),\mathbf{c}$	$x-y,x+y,z+\frac{1}{4}$	$x-y,x+y,z$	$8b$	$16e$	$16c$	$8a;16f$	$32g$ $16e;32g$	$16d;2\times16f$ $3\times32g$
	conjugate: $\frac{1}{2}(\mathbf{b}-\mathbf{c}),\frac{1}{2}(\mathbf{b}+\mathbf{c}),\mathbf{a}$	$y-z,y+z,x+\frac{1}{4}$	$y-z,y+z,x$						
	conjugate: $\frac{1}{2}(-\mathbf{a}+\mathbf{c}),\frac{1}{2}(\mathbf{a}+\mathbf{c}),\mathbf{b}$	$-x+z,x+z,y+\frac{1}{4}$	$-x+z,x+z,y$						
II Maximal *klassengleiche* subgroups									
Enlarged unit cell, isomorphic									
[27] $Fd\bar{3}c$	$3\mathbf{a},3\mathbf{b},3\mathbf{c}$	$\underbrace{\frac{1}{3}x+\frac{1}{4},\frac{1}{3}y+\frac{1}{4},\ \frac{1}{3}z+\frac{1}{4};}$ $\pm(\frac{1}{3},0,0);\pm(0,\frac{1}{3},0);\pm(0,0,\frac{1}{3});$ $\pm(0,\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},0,\frac{1}{3});\pm(\frac{1}{3},\frac{1}{3},0);$ $\pm(0,\frac{1}{3},\frac{2}{3});\pm(\frac{1}{3},0,\frac{2}{3});\pm(\frac{1}{3},\frac{2}{3},0);$ $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3});\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3});$ $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$\frac{1}{3}x,\frac{1}{3}y,\frac{1}{3}z;$	$16a;$ $2\times64e;$ $96f;192h$	$32b;64e;$ $2\times96g;$ $3\times192h$	$32c;64e;$ $4\times192h$	$48d;96f;$ $6\times192h$	$3\times64e;$ $8\times192h$ $3\times96g;$ $12\times192h$	$3\times96f;$ $12\times192h$ $27\times192h$

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International Tables for Crystallography (2006). Vol. A1, Wyckoff relations for space group 229, pp. 720–721.

$Im\bar{3}m$ No. 229 $I\,4/m\,\bar{3}\,2/m$ O_h^9

Subgroup	Axes	Coordinates	2a	6b	8c 24h	12d 48i	12e 48j	16f 48k	24g 96l
I Maximal *translationengleiche* subgroups									
[2] $I\bar{4}3m$ (217)			2a	6b	8c 24g	12d 48h	12e 48h	2×8c 2×24g	24f 2×48h
[2] $I432$ (211)			2a	6b	8c 24h	12d 2×24i	12e 48j	16f 48j	24g 2×48j
[2] $Im\bar{3}$ (204)			2a	6b	8c 24g	12e 48h	12d 2×24g	16f 48h	2×12e 2×48h
[4] $R\bar{3}m$ (166)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	1a	3e	1b; 3d 6f; 6h	6g 2×6g; 12i	6h 2×12i	2c; 6h 2×6h; 12i	12i 4×12i
	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}, \frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x+y+z), \frac{1}{3}(-x-y+2z), \frac{2}{3}(x+y+z)$	3a	9e	3b; 9d 18f; 18h	18g 2×18g; 36i	18h 2×36i	6c; 18h 2×18h; 36i	36i 4×36i
	conjugate: $\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x+y-z), \frac{1}{3}(x-y-2z), \frac{2}{3}(-x+y-z)$							
	conjugate: $-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}, \frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(-2x-y-z), \frac{1}{3}(-x+y-2z), \frac{2}{3}(x-y-z)$							
	conjugate: $\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}, \frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hexagonal axes)	$\frac{1}{3}(2x-y+z), \frac{1}{3}(x+y+2z), \frac{2}{3}(-x-y+z)$							
[3] $I4/mmm$ (139)			2a	2b; 4c	8f 8h; 16n	4d; 8j 16k; 32o	4e; 8i 16l; 2×16n	16m 16m; 32o	8g; 2×8j 3×32o
	conjugate: $\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x							
	conjugate: $\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y							
II Maximal *klassengleiche* subgroups									
Loss of centring translations									
[2] $Pn\bar{3}m$ (224)		origin 1: x, y, z origin 2: $x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	2a	6d	4b; 4c 24k	12f 24i; 24j	12g 48l	2×8e 2×24k	24h 2×48l
[2] $Pm\bar{3}n$ (223)			2a	6b	8e 24k	6c; 6d 2×24j	12f 2×24k	16i 48l	12g; 12h 2×48l
[2] $Pn\bar{3}n$ (222)		origin 1: x, y, z origin 2: $x+\frac{1}{4}, y+\frac{1}{4}, z+\frac{1}{4}$	2a	6b	8c 24h	12d 48i	12e 48i	16f 48i	24g 2×48i
[2] $Pm\bar{3}m$ (221)			1a; 1b	3c; 3d	8g 12i; 12j	12h 48n	6e; 6f 24k; 24l	2×8g 2×24m	2×12h 2×48n
Enlarged unit cell, isomorphic									
[27] $Im\bar{3}m$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	2a; 12e; 16f; 24h	6b; 12e; 24g; 24h; 48j; 48k	8c; 16f; 48i; 3×48k 3×24h; 3×48j; 3×48k; 3×96l	12d; 24g; 48i 3×48j; 96l 3×48i; 12×96l	3×12e; 3×48j; 3×48k 9×48j; 9×96l	3×16f; 6×48k; 96l 9×48k; 9×96l	3×24g; 6×48j; 3×96l 27×96l

	Axes	Coordinates	Wyckoff positions					
			$2a$ $24g$	$6b$ $24h$	$8c$ $48i$	$12d$ $48j$	$12e$ $48k$	$16f$ $96l$
$[p^3]\,Im\bar{3}m$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ $p = \text{prime} > 2$; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$2a; \frac{p-1}{2}\times 12e$; $\frac{p-1}{2}\times 16f$; $\frac{p-1}{2}\times 24h$; $\frac{(p-1)(p-3)}{8}\times 48j$; $\frac{(p-1)(p-3)}{4}\times 48k$; $\frac{(p-1)(p-3)(p-5)}{48}\times 96l$	$6b; \frac{p-1}{2}\times 12e$; $\frac{p-1}{2}\times 24g$; $\frac{p-1}{2}\times 24h$; $\frac{(p-1)(3p-5)}{8}\times 48j$; $\frac{(p-1)^2}{4}\times 48k$; $\frac{(p-1)^2(p-3)}{16}\times 96l$	$8c; \frac{p-1}{2}\times 16f$; $\frac{p-1}{2}\times 48i$; $\frac{p(p-1)}{2}\times 48k$; $\frac{(p^2-1)(p-3)}{12}\times 96l$	$12d; \frac{p-1}{2}\times 24g$; $\frac{p-1}{2}\times 48i$; $\frac{p(p-1)}{2}\times 48j$; $\frac{(p^2-1)(p-2)}{8}\times 96l$	$p\times 12e$; $\frac{p(p-1)}{2}\times 48j$; $\frac{p(p-1)}{2}\times 48k$; $\frac{p(p-1)(p-3)}{8}\times 96l$	$p\times 16f$; $p(p-1)\times 48k$; $\frac{p(p-1)(p-2)}{6}\times 96l$
			$p\times 24g$; $p(p-1)\times 48j$; $\frac{p(p-1)^2}{4}\times 96l$	$p\times 24h$; $\frac{p(p-1)}{2}\times 48j$; $\frac{p(p-1)}{2}\times 48k$; $\frac{p(p-1)^2}{4}\times 96l$	$p\times 48i$; $\frac{p(p^2-1)}{2}\times 96l$	$p^2\times 48j$; $\frac{p^2(p-1)}{2}\times 96l$	$p^2\times 48k$; $\frac{p^2(p-1)}{2}\times 96l$	$p^3\times 96l$

$Ia\bar{3}d$ No. 230 $I4_1/a\bar{3}2/d$ O_h^{10}

	Axes	Coordinates	Wyckoff positions $16a$	 $16b$	 $24c$	 $24d$	 $32e$ $48g$	 $48f$ $96h$
I Maximal *translationengleiche* subgroups								
[2] $I\bar{4}3d$ (220)			$16c$	$16c$	$24d$	$12a; 12b$	$2\times16c$ $48e$	$2\times24d$ $2\times48e$
[2] $I4_132$ (214)			$16e$	$8a; 8b$	$12c; 12d$	$24f$	$2\times16e$ $24g; 24h$	$2\times24f$ $2\times48i$
[2] $Ia\bar{3}$ (206)			$8a; 8b$	$16c$	$24d$	$24d$	$2\times16c$ $48e$	$2\times24d$ $2\times48e$
[4] $R\bar{3}c$ (167)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$y+z, x+z, x+y$ (rhombohedral axes)	$2b; 6d$	$2a; 6e$	$2\times6e$	$12f$	$4c; 12f$ $2\times6e; 12f$	$2\times12f$ $4\times12f$
	$-\mathbf{a}+\mathbf{b}, -\mathbf{b}+\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ (hex. axes)	$\frac{1}{3}(-2x+y+z)$, $\frac{1}{3}(-x-y+2z)$, $\frac{2}{3}(x+y+z)$	$6b; 18d$	$6a; 18e$	$2\times18e$	$36f$	$12c; 36f$ $2\times18e; 36f$	$2\times36f$ $4\times36f$
conjugate:	$\mathbf{a}+\mathbf{b}, -\mathbf{b}-\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{b}-\mathbf{c})$ (hex. axes)	$\frac{1}{3}(2x+y-z)$, $\frac{1}{3}(x-y-2z)+\frac{1}{2}$, $\frac{2}{3}(-x+y-z)$						
conjugate:	$-\mathbf{a}-\mathbf{b}, \mathbf{b}-\mathbf{c}$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}-\mathbf{c})$ (hex. axes)	$\frac{1}{3}(-2x-y-z)+\frac{1}{2}$, $\frac{1}{3}(-x+y-2z)$, $\frac{2}{3}(x-y-z)$						
conjugate:	$\mathbf{a}-\mathbf{b}, \mathbf{b}+\mathbf{c}$, $\frac{1}{2}(-\mathbf{a}-\mathbf{b}+\mathbf{c})$ (hex. axes)	$\frac{1}{3}(2x-y+z)-\frac{1}{2}$, $\frac{1}{3}(x+y+2z)-\frac{1}{2}$, $\frac{2}{3}(-x-y+z)$						
[3] $I4_1/acd$ (142)		origin 1: $x, y-\frac{1}{4}, z+\frac{1}{8}$ origin 2: x, y, z	$16c$	$16f$	$8b; 16e$	$8a; 16e$	$32g$ $16f; 32g$	$16d; 2\times16e$ $3\times32g$
conjugate:	$\mathbf{b}, \mathbf{c}, \mathbf{a}$	y, z, x (origin 2)						
conjugate:	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	z, x, y (origin 2)						
II Maximal *klassengleiche* subgroups								
Enlarged unit cell, isomorphic								
[27] $Ia\bar{3}d$	$3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$	$\frac{1}{3}x, \frac{1}{3}y, \frac{1}{3}z$; $\pm(\frac{1}{3},0,0)$; $\pm(0,\frac{1}{3},0)$; $\pm(0,0,\frac{1}{3})$; $\pm(0,\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},0,\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},0)$; $\pm(0,\frac{1}{3},\frac{2}{3})$; $\pm(\frac{1}{3},0,\frac{2}{3})$; $\pm(\frac{1}{3},\frac{2}{3},0)$; $\pm(\frac{1}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{2}{3},\frac{1}{3})$; $\pm(\frac{1}{3},\frac{1}{3},\frac{2}{3})$	$16a; 32e;$ $4\times96h$	$16b; 32e;$ $2\times48g;$ $3\times96h$	$24c; 48f;$ $2\times48g;$ $5\times96h$	$24d; 48f;$ $6\times96h$	$3\times32e;$ $8\times96h$ $3\times48g;$ $12\times96h$	$3\times48f;$ $12\times96h$ $27\times96h$
[p^3] $Ia\bar{3}d$	$p\mathbf{a}, p\mathbf{b}, p\mathbf{c}$ p = prime > 2; $u, v, w = 1, \ldots, p-1$	$\frac{1}{p}x, \frac{1}{p}y, \frac{1}{p}z$; $+(\frac{u}{p}, \frac{v}{p}, \frac{w}{p})$	$16a;$ $\frac{p-1}{2}\times32e;$ $\frac{p(p^2-1)}{6}\times96h$	$16b;$ $\frac{p-1}{2}\times32e;$ $(p-1)\times48g;$ $\frac{p^3-4p+3}{6}\times96h$	$24c;$ $\frac{p-1}{2}\times48f;$ $(p-1)\times48g;$ $\frac{(p-1)^2(p+2)}{4}\times96h$	$24d;$ $\frac{p-1}{2}\times48f;$ $\frac{p(p^2-1)}{4}\times96h$	$p\times32e;$ $\frac{p(p^2-1)}{3}\times96h$ $p\times48g;$ $\frac{p(p^2-1)}{2}\times96h$	$p\times48f;$ $\frac{p(p^2-1)}{2}\times96h$ $p^3\times96h$

APPENDIX
Differences in the presentation of Parts 2 and 3

BY ULRICH MÜLLER AND HANS WONDRATSCHEK

A1. Comparison of the approaches to subgroups in Parts 2 and 3

The tables in Parts 2 and 3 of this volume deal with two different aspects of the reduction of crystal symmetry. In Part 2, the loss of symmetry is described for the subgroup $\mathcal{H}$ of $\mathcal{G}$ by listing the *general position* of $\mathcal{H}$, *i.e.* a set of representatives of those symmetry operations (group elements) which are retained in $\mathcal{H}$. If there is not enough space to include the full general position, at least a set of generators of $\mathcal{H}$ is listed. Thus, the subject of Part 2 is *symmetry*. In Part 3, the splitting of the point orbits (*Wyckoff positions*) of the space group $\mathcal{G}$ when the symmetry of $\mathcal{G}$ is reduced to that of $\mathcal{H}$ is described. For each Wyckoff position of $\mathcal{G}$ the corresponding Wyckoff positions of $\mathcal{H}$ are listed. Thus, in Part 3 the *implications of symmetry changes for crystal structures* are described.

In both Parts 2 and 3, the data are listed in a way that makes the tables as convenient to use as possible. As the subjects of Parts 2 and 3 are different, the presentation of the data in the two parts differs. In addition, the data in Part 2 are such that they can be used more-or-less independently from Volume A of *International Tables for Crystallography* (2002) (abbreviated as *IT* A). This independence is not possible for the data in Part 3.

In order to facilitate the combined use of the data in the two parts, the differences in the presentation of these data are summarized in this Appendix.

A2. Multiple descriptions of the space groups $\mathcal{G}$ and $\mathcal{H}$

In *IT* A, some space groups are described up to six times:

(i) all monoclinic space groups are referred to unique axis *b* and unique axis *c*; for most of them a further partition is made into cell choice 1, cell choice 2 and cell choice 3;

(ii) 24 orthorhombic, tetragonal and cubic space groups are referred to origin choice 1 and origin choice 2;

(iii) seven space groups with rhombohedral lattice are referred to hexagonal axes and rhombohedral axes.

Multiple descriptions of the space group $\mathcal{G}$ are treated differently in Parts 2 and 3 of this volume:

(i) In Part 2, the data for each monoclinic space group $\mathcal{G}$ are listed for unique axis *b* and unique axis *c* on separate pages, but both for cell choice 1 only. In Part 3, the description is more explicit: for each setting unique axis *b* or unique axis *c* with different cell choices in *IT* A, the subgroups are listed for cell choice 1, cell choice 2 and cell choice 3.

(ii) In Part 2, the data for origin choice 1 and origin choice 2 are listed on separate pages. In Part 3, the data for both origin choices are combined on the same page.

(iii) In Part 2, descriptions in both hexagonal axes and rhombohedral axes are given; in Part 3 only a description in hexagonal axes is presented.

Multiple descriptions of the subgroup $\mathcal{H}$ are also sometimes treated differently in the two parts:

(i) The treatment of monoclinic subgroups is broadly the same: if the subgroup is given in a conventional setting (unique axis *b* or unique axis *c*), then this setting is kept. Otherwise, an nonconventional setting is transformed to unique axis *b*. However, in Part 3 the treatment is more explicit and adapted to the practice of crystal-structure description: in some cases several possible choices of axes transformations are listed for the same monoclinic subgroup. It is hoped that one of them corresponds to the cell with the commonly preferred metric values. The different possibilities are indicated by the words 'or' or 'alternative', *e.g.* for the monoclinic subgroup $P112_1/m$, No. 11, of *Cmcm*, No. 63, *cf.* also Section 3.1.6 (p. 433).

(ii) The treatment of two origin choices is the same with one exception: if only $\mathcal{H}$ is listed with two origins in *IT* A, then in Part 2 only the data for origin choice 2 are provided, while in Part 3 the data for both origin choices are listed.

(iii) The treatment of rhombohedral subgroups $\mathcal{H}$ is broadly similar. The subgroup is referred to hexagonal axes with two exceptions:

(*a*) in Part 2 the setting of the subgroup $\mathcal{H}$ is rhombohedral if the setting of $\mathcal{G}$ is rhombohedral (this does not apply to Part 3);

(*b*) in Part 3, for the rhombohedral subgroups of cubic space groups both settings are given, whereas in Part 2 only the hexagonal-axes setting is referred to.

A3. The transformation matrix and the origin shift

When starting from a space group $\mathcal{G}$ and proceeding to one of its subgroups $\mathcal{H} < \mathcal{G}$, the symmetry operations and the point coordinates are primarily referred to the coordinate system of $\mathcal{G}$. This coordinate system consists of a coordinate basis of three linearly independent basis vectors and an origin. In general, the conventional coordinate system of $\mathcal{H}$ will not be identical to that of $\mathcal{G}$ but the transition from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$ may involve a change of the basis and an origin shift. This transition or coordinate transformation is not uniquely determined but may be chosen within certain limits. The optimal choice will be the coordinate transformation that is the most convenient and easy for the user to work with.

For the following, it is assumed that the original crystal structure and its space group $\mathcal{G}$ and symmetry operations are referred to a conventional coordinate system, because the data in the tables of this volume and in *IT* A are listed under this condition. Otherwise, a coordinate transformation to a conventional coordinate system has to precede the use of most of the data. The coordinate transformation itself is described by the matrix $\boldsymbol{P}$ of the coefficients of the basis vectors of the new basis referred to the old basis and by a column $\boldsymbol{p}$ which consists of the coordinates of the new origin referred to the old coordinate system, *cf.* Section 2.1.3 (p. 45) or, more explicitly, *IT* A, Part 5. The matrix $\boldsymbol{P}$ is presented in Parts 2 and 3 by listing the new basis vectors as linear combinations of the old ones, *e.g.* $(\mathbf{a}' =)\ \mathbf{a} - \mathbf{b}$, $(\mathbf{b}' =)\ \mathbf{a} + \mathbf{b}$, $(\mathbf{c}' =)\ \mathbf{c}$. The column $\boldsymbol{p}$ is presented in Part 2 by listing the coefficients of the shift vector, *e.g.* $0, 1/2, 1/4$. For Part 3, the representatives of the Wyckoff positions are taken as triplets of point coordinates. The transformation behaviour of coordinates is different from that of the symmetry operations, *viz* $\boldsymbol{x}' = \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p})$, where $\boldsymbol{x}$ and $\boldsymbol{x}'$ are the coordinate columns of the points of the crystal structure in the old and in the new coordinate systems.

The criteria for selecting the coordinate transformations are different in Parts 2 and 3. In Part 2, emphasis is placed on homogeneity by using similar transformation matrices in similar situations. In Part 3, the preferred transformation is that which avoids an origin shift, *i.e.* for which the resulting shift vector is the **o** vector.

Example.

In the relation

$$I4_1/amd\ (141) \to Fddd(70)$$

the axes must be transformed, either by $\mathbf{a}-\mathbf{b},\ \mathbf{a}+\mathbf{b},\ \mathbf{c}$ or by $\mathbf{a}+\mathbf{b},\ -\mathbf{a}+\mathbf{b},\ \mathbf{c}$. If origin choice 1 is selected for both space groups, then the first of these transformations requires an origin shift of $0, 1/2, 1/4$ (referred to the coordinate system of $I4_1/amd$). The first transformation is used in Part 2 because in all such relations the new basis of $\mathcal{H}$ is rotated against the old basis of $\mathcal{G}$ by a clockwise rotation of 45° and the necessary origin shift is then accepted. No origin shift is needed for the second transformation and, therefore, it has been used in Part 3; this can be seen in the transformation of the coordinates:

$$(x' =)\ \tfrac{1}{2}(x+y),\ (y' =)\ \tfrac{1}{2}(-x+y),\ (z' =)\ z.$$

Another difference between Parts 2 and 3 concerns the origin shifts chosen and their presentation. The common point of view is to make the origin shift positive unless special conditions lead to a preference for negative coefficients. However, the shift vector **s** of Part 3 is calculated by $\mathbf{s} = -\boldsymbol{P}^{-1}\mathbf{p}$ from the shift vector **p** of Part 2, so the two vectors usually have opposite directions. Therefore, very often a positive shift vector in Part 2 corresponds to a negative shift vector in Part 3 and *vice versa*. This is not obvious at first glance, because in Part 2 the vector **p** is listed, whereas in Part 3 the shift vector is given as part of the coordinate transformations.

Example.

Consider *Pccn*, No. 56, as a subgroup of *Cccm*, No. 66, in the block 'Loss of centring translations'. The origin shift $1/4, 1/4, 0$ of Part 2 has the opposite direction to that of Part 3, where it is indicated as part of the transformation '$x+\frac{1}{4}, y+\frac{1}{4}, z(+0)$'. The components $\frac{1}{4}, \frac{1}{4}, 0$ of this transformation correspond to a vector $\mathbf{p} = (-\frac{1}{4}, -\frac{1}{4}, 0)$, which is the opposite of the vector **p** of Part 2.

Since the Wyckoff letters of the positions in *IT* A may depend not only on the chosen basis but also on the chosen origin, a difference in the origin shift may induce a difference in the relations between the Wyckoff positions.

Example.

Consider $P4_2/m$, No. 84, as a *translationengleiche* subgroup of $P4_2/mnm$, No. 136. The coordinate transformation $x+\frac{1}{2}, y, z$ of Part 3 results in the relations $2a \longrightarrow 2d$ and $2b \longrightarrow 2c$ of the Wyckoff positions. The origin shift $0, 1/2, 0$ of Part 2 (which corresponds to a coordinate transformation $x, -\frac{1}{2}+y, z$) results in the relations $2a \longrightarrow 2c$ and $2b \longrightarrow 2d$.

A4. Nonconventional settings

If the setting of a subgroup is nonconventional, in Part 2, as in *IT* A, an nonconventional Hermann–Mauguin symbol is listed referred to the basis of $\mathcal{G}$, followed by the space-group number and the conventional symbol in parentheses. In Part 3, nonconventional settings are given only by Hermann–Mauguin symbols that correspond to the conventions of the crystal system followed on the next line by $\widehat{=}$ and the symbol of the conventional setting.

Examples.

	Subgroup entry in Part 2	Subgroup entry in Part 3
Space group $P222$, No. 16	$A222$ (21, $C222$)	$A222$ (21) $\widehat{=}\, C222$
Space group $I4_122$, No. 98	$I2_112$ (22, $F222$)	$F222$ (22)

In Part 3, unlike Part 2, no use is made of centred triclinic cells, *F*- and *R*-centred monoclinic cells, *C*- and *F*-centred tetragonal cells and *H*-centred hexagonal cells.

A5. The sequence of the subgroups

The sequence of the subgroups follows the same principles in both parts. The *translationengleiche* subgroups are listed first, the *klassengleiche* subgroups follow. The subgroups are distributed into blocks; within the same block the index generally determines the sequence (lower index precedes higher index). For the same index, the space-group number determines the sequence (higher space-group number precedes lower space-group number). A difference in the sequence is caused by two special rules that apply to Part 3:

(i) The sequence of the *translationengleiche* subgroups of cubic space groups does not follow the index value, but is in the order cubic, rhombohedral, tetragonal, orthorhombic.

(ii) The last *translationengleiche* subgroup of a tetragonal space group is always the one with the diagonally oriented cell, irrespective of its space-group number.

The sequence of the listings of the *klassengleiche* subgroups differs more often, because the partition of the subgroups into blocks in Part 2 is different from and finer than that in Part 3. The blocks in Part 2 are determined by the relation of the lattice of $\mathcal{H}$ to that of $\mathcal{G}$, *i.e.* by the different kinds of cell enlargement, and the index and space-group numbers are decisive for the sequence within these (small) blocks only.

The isomorphic subgroups are placed differently in Parts 2 and 3. Those with index values of 2, 3 and 4 are listed in Part 2 together with the other *klassengleiche* subgroups; they may also be contained in the infinite series of isomorphic subgroups that follow. In Part 3, all isomorphic subgroups are listed in a separate block.

A6. Conjugate subgroups

Conjugate subgroups are listed in Part 3 only in the case of orientational conjugation, *cf.* Section 3.1.5.2 (p. 433). They are marked by the word 'conjugate'. In Part 2, all conjugate subgroups of index 3 and 4 are listed individually and are joined by a left brace. In the series of maximal isomorphic subgroups, the conjugacy relations are given by statements.

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