**Nmr Experiment Nomenclature v2 (2011)**

**Data model for experiment description**

Nmr Experiment Prototypes are described in the[ccp.nmr.NmrExpPrototype](https://www2.ccpn.ac.uk/api-documentation/ccpnmr/ccpnmr2.2/python/ccp/api/doc/nmr/NmrExpPrototype/index.html) package of the data model. For details and diagrams please follow the link.

Experiment descriptions are organised in NmrExpPrototypesthat each describes a magnetisation transfer pathway and the NMR experiments that use it. The nuclei involved in the magnetisation transfer are described by AtomSites, with information like isotope, allowed chemical shift ranges, and multiplicities. ExpMeasurements describe the quantities measured in the experiments. In most cases there is a single ExpMeasurement for each AtomSite, which corresponds to the chemical shift. Other possibilities include coupling constants, relaxation times, or multiple quantum shifts. The magnetisation flow in the experiment is described by the ExpGraph and associated objects. ExpTransfer objects show which kinds of magnetisation transfer link the AtomSites, while the sequence of ExpSteps show the flow of magnetisation during the experiment. There can be more than one ExpGraph for experiments that include more than one magnetisation flow. An example is the HCBCACONNH experiment, where magnetisation may start on either Hβ or Hα. The recognised transfer types are: 'onebond' ,'Jcoupling', 'Jmultibond', 'relayed', 'through-space', and 'relayed-alternate' . The RefExperiment and associated objects describes the number of dimensions in the actual experiment, which quantities are measured, and how the measurements map onto the experiment axes. There can be more than one measurement per axis for projection experiments, or for experiments that measure e.g. 13C and 15N evolution in parallel on a single axis. RefExperiments where the magnetisation flow is reversed are part of the same NmrExpPrototype – e.g. HcanHA and HncaHA are both included in the HNCAHA NmrExpPrototype.

Experiment descriptions are meant to reflect the possible assignments for peaks and must ultimately be chosen by the spectroscopist. The appropriate description cannot be deduced from the pulse sequence alone. For instance choosing the CC reference experiment implies that only peaks between directly bound carbons are possible in the specific experiment. In this context it is irrelevant whether the pulse sequence might have given rise to other kinds of peaks with a different choice of mixing time, or if applied to a different sample.

**Nmr Experiment Nomenclature**

NMR experiment names are built on the corresponding description in the CCPN data model. As such they are unambiguous and reflect the network of nuclei and the flow of magnetisation between them, but not the physical transfer processes involved. The naming system has been chosen to conform to the common naming style for experiments to the extent allowed by these requirements.

Naming Rules

* 1. The naming convention is the same for NmrExpPrototypes (describing magnetisation transfer pathways) and RefExperiments (describing a specific experiment using the pathway). The name of the NmrExpPrototype must be the same as the name of the highest dimensionality non-reversed RefExperiment.
  2. Experiments are normally named by concatenating the names of the AtomSites in the order that the atoms are traversed during the experiment (e.g. **HCACONH**). If there are no further restrictions on the AtomSite it is given the name of the relevant nucleus. Thus 'N' means 'any 15N', 'C' means 'any 13C' etc. Longer names can be used to identify specific types of nucleus, provided that names for proton sites start with H, those for carbon sites with C, etc. The names 'CO' (carbonyl), 'Cali' (aliphatic carbon), 'Caro' (aromatic carbon) and 'Cmet' (methyl carbon) have a conventional meaning; other names (like CA, CB, …) have a specific meaning in certain subfields, e.g. protein NMR. Experiment names should reflect the kind of peaks that the experiment measures, but the name of each AtomSite can be chosen flexibly. The **HNCAHA** experiment (for instance) must be selective for the alpha position in some way – otherwise it would be no different from the HN\_CH.Jcoupling experiment - but the AtomSite name 'HA' does not imply that the proton frequency is excited selectively.
  3. Parts of the magnetisation transfer network that are measured are in upper case, while parts that are not measured are in lower case. Thus:  
     + **HCACONH** (5D experiment, also the name of the NmrExpPrototype)
     + **HcacoNH** (H(CACO)NNH, a 3D 1H,15N,1H experiment).
     + **hCAcoNH** ((H)CA(CO)NNH, a 3D 13C,15N,1H experiment).
  4. The experiment name also reflects the magnetisation transfer types. The allowed types are 'onebond' ,'Jcoupling', 'Jmultibond', 'relayed', 'through-space', and 'relayed-alternate'. The default transfer type is 'onebond', except for couplings between hydrogens and/or halogens, where the default is 'Jcoupling'. For transfer between atoms ‘N’ and ‘CA’ the default is also 'Jcoupling', and onebond transfer must be indicated explicitly – this is an exception that allows experiment names like HNCAHA to retain their accepted meaning. Transfer types that differ from the default are indicated by putting an underscore at the place of the transfer, and listing the transfer types at the end of the experiment name, in order. The following examples show the format:  
     + **H\_H.through-space** (1H NOESY);
     + **HC\_CH.relayed** (HCCH-TOCSY);
     + **CA\_NCO.onebond** (CANCO),
     + **Cali\_Cali\_C.relayed,through-space**(carbon 3D, with relayed magnetisation transfer between two aliphatic carbons, followed by through-space transfer to a third carbon).
  5. In many experiments the magnetisation transfer pathway is not linear but contains out-and-back segments. These are indicated by putting the out-and-back trace in square brackets:  
     + **H[N]\_H.through-space**(15N HSQC-NOESY)
     + **H\_[C].Jmultibond** (carbon-proton correlation through weak, long-range couplings)
     + **H[C]\_H[C].through-space**(4D 13C,13C HSQC-NOESY-HSQC).
  6. Some experiments exist in both out-and-back and straight-through versions; for instance **HNCAHA**is an experiment that starts on H and ends on HA, whereas the out-and-back version is called **H[N[CA[HA]]].**
  7. Filtered experiments select atoms on the basis of their couplings without necessarily transferring the magnetisation to the coupling partners. Thus:  
     + **H[C[co]]** (2D 13C HSQC selecting carbons bound to carbonyl).
     + **HCC[h(0)]**(3D relayed inept, selecting quaternary carbons)
  8. Some, mainly filtered, experiments select on multiplicity. Here the allowed number of atoms is added in parenthesis. Thus:
     + **H[C[h(2n+1)]]** (13C HSQC selecting CH and CH3 groups)
     + **H[N[h(2n)]]** (15N HSQC selecting NH2 (and NH4) groups)
     + **CH(1)** (idept-90 – 2d 13C -excited, 1H -detected correlation selecting CH groups)
  9. Some experiments include parallel magnetisation flows, which are indicated by curly braces. The simplest case is that of concurrent flow through a single transfer network, where it does not make sense to specify the order in which certain steps are traversed. Such steps are separated by a plus sign. Thus:  
     + **H{[N]+[HA]}** (The HNHA experiment for coupling measurement. Transfer to N and HA is simultaneous).
     + **H{[n(0)]+[c(0)]}\_H.through-space** (NOESY, selecting protons not bound to labelled carbon or nitrogen in dimension 1).
  10. The more common case is when the experiment allows several alternative magnetisation transfer flows. Here alternative flows are separated by a pipe character ('|'):  
      + **H[{N|C}]\_H.through-space** (3D combined 13C and 15N HSQC-NOESY)
      + **H{CA|Cca}NH** (4D HBCB/HACANNH, straight-through version. Magnetisation flow is either HBCBCANH or HACANH...)
      + **H[N[{CA[H]|ca[C[H]]}]]** (4D HNCAHA/CBHB, out-and-back version)
  11. Sometimes alternative magnetisation pathways are distinguished because they give rise to different peak signs. Thus:  
      + **{H(2n+1)|H(2n)}C** (deptq-135 – 2D proton-excited, carbon-detected correlation with opposite sign for CH/CH3 and C/CH2, with quaternary carbons included)
      + **{H(2n+1)|H(2)}[C]\_H.relayed** (HSQC-TOCSY with opposite sign for CH2 and CH2N+1)
  12. Magnetisation may pass through other states than single quantum shifts. These are represented by giving the measurement type, with the nuclei involved in parenthesis:  
      + **C[DQ(CC)]** (2D carbon double quantum spectroscopy)
      + **H[{J(HH)|J(CH)}]**(2D J-resolved, measuring proton-proton and proton-carbon couplings)
      + **H[T1(H)]** (1D 1H T1)
      + **H[N[T2(N)][CO]]** (HNCO measuring T2(N))
      + **H[N][T1rho(H)]** (15N HSQC – 1H T1 rho)
      + **H[N][T1zz(HN)]** (15N HSQC – 1H-15N T1zz)
  13. Experiments of three dimensions and higher may be acquired as projection experiments. In these a number of delays are incremented in a coordinated manner, rather than independently, so that several experimental axes are collapsed into one. The magnetisation along the resulting axis evolves as a linear combination of the evolutions that would have occurred along the original axes. The projection experiments used in practice tend to have two dimensions, with all non-acquisition axes included in the projection. Experiments are acquired as a number of different linear combinations, which may include one or more of the projected axes.
  14. Projection experiments are named by combining the name of the unprojected experiment, the dimensionality of the resulting experiment, and the names of the axes involved in the projection. To reduce the number of reference descriptions necessary, it is recommended to use a single experiment with the highest possible number of axes in the projection, even if not all these axes are exercised in a specific experiment. The format can be seen from the examples. All are 2D projections:  
      + **H[CA[CO[N]]].2D.{CA;CO;N}** (out-and-back 4D HCACON)
      + **HC\_caNH.relayed.2D.{H;C;N}** (4D HC-TOCSY-CNH)
      + **Hnca\_CH.relayed.2D.{H;N;C}**(4D HNC-TOCSY-CH - reverse of the preceding experiment)
      + Explanatory text may be added – sparingly – at the start of the name, followed by a dot. E.g.:
      + **ct.H[C[{cali(2n)|cali(2n+1)}]]** (constant-time carbon HSQC with opposite peak sign according to the odd/even number of aliphatic carbon coupling partners)
      + **seq.H[N[CA]]**(sequential-only HNCA, measuring only the Cαi-1)
  15. Spaces in names are discouraged, but may be added for clarification in particularly complex cases. An example is the 2D double-half filtered labelled<->unlabelled NOESY, currently the experiment with the most complex name. It also exemplifies several of the points in paragraph 8). It is named:
      + **{ H[{n|c}]\_H{[n(0)+c(0)]} | H{[n(0)+c(0)]}\_H[{n|c}] }.through-space**