NMR-STAR save frame groupings and save frame categories

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| **Table S2.** NMR-STAR save frame groupings and save frame categories | | |
| **Super category group** | **Category group** | **Description** |
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| entry\_information |  | Information describing the entry, any study that the entry is a member, and information regarding the processing of the entry and updates to the entry after its initial release to the public. |
|  | study\_list | Categories that describe a study of a molecular system that includes data from one or more entries. |
|  | entry\_information | Categories that describe an entry. |
|  | deposited\_data\_files | Categories that capture information about the data files that are uploaded for depositions. |
|  | entry\_interview | Categories that record an overview of the information to be deposited by an author. |
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| citations |  | Citations referenced in the entry and the primary citation related to this specific entry. |
|  | citations | Categories that provide detailed easily searched data on bibliographic references, in particular the citation directly related to the data in a entry. |
|  | reference (proposed) | Categories that provide bibliographic references in a format similar to that found in a publication. |
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| assembly\_supercategory |  | The assembly\_supercategory contains the complete chemical description of the molecular assembly studied, additional reference information for the molecular assembly and its components, and links to information for the equivalent or similar molecular assemblies or biopolymer components in other databases. |
|  | assembly | Categories that describe a molecular assembly. |
|  | assembly\_annotation | Categories that provide annotations for a molecular assembly. |
|  | assembly\_subsystems | Categories that describe subsystems of a molecular assembly. |
|  | entity | Categories that describe the polymer and non-polymer  molecules that make up a molecular assembly. |
|  | natural\_source | Categories that describe the organism or other body found  in nature that produces a molecular entity. |
|  | experimental\_source | Categories that describe the system used to produce a  molecular entity for scientific experiments. |
|  | chem\_comp | Categories that describe chemical components of entities  and molecular assemblies. |
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| experimental\_details |  | The experimental\_details category super group captures information about the samples, sample conditions, NMR spectrometers, NMR experiments and other data regarding the experiments used to collect the NMR spectral  data and to derive kinetic, thermodynamic, and structure information. |
|  | sample | Categories that describe the contents and other details about the samples used in scientific experiments. |
|  | sample\_conditions | Categories that describe the experimental conditions used in conducting individual scientific experiments. |
|  | molecule\_purity | Categories that describe the measured purity of a molecular entity. |
|  | software | Categories that describe computer software. |
|  | software\_specific\_saveframes | Categories that capture as a block of text a STAR save frame generated by a software application that is not an NMR-STAR compliant save frame. |
|  | applied\_software | Categories that describe in some detail the software scripts and parameters used in creating the data reported in an entry. |
|  | applied\_software\_history | Categories that define the order and how software tools are applied in generating the reported data. |
|  | method | Categories that describe software or physical methods used to produce a product. |
|  | Mass\_spectrometer | Categories that describe a mass spectrometer. |
|  | Mass\_spectrometer\_list | Categories that describe a list of mass spectrometers and their properties. |
|  | Mass\_spec\_ref\_compd | Categories that describe reference compounds used to calibrate mass spectral data. |
|  | Chromatographic\_system | Categories that describe a chromatographic system. |
|  | Chromatographic\_column | Categories that describe a chromatographic column. |
|  | fluorescence\_instrument | Categories that describe a fluorescence instrument. |
|  | EMR\_instrument | Categories that describe an EMR instrument. |
|  | Xray\_instrument | Categories that describe a X-ray instrument. |
|  | NMR\_spectrometer | Categories that describe an NMR spectrometer. |
|  | NMR\_spectrometer\_list | Categories that define a list of NMR spectrometers and their properties. |
|  | NMR\_spectrometer\_probe | Categories that describe an NMR spectrometer probe. |
|  | NMR\_spectrometer\_expt\_list | Categories that define a list of NMR spectrometer experiments. |
|  | NMR\_spectrometer\_expt | Categories that describe an NMR spectrometer experiment in detail. |
|  | NMR\_spectral\_processing | Categories that describe how the data from an NMR spectrometer experiment has been processed. |
|  | Experiment\_list | Categories that describe a list of experiments. |
|  | MS\_expt | Categories that describe a mass spectroscopy experiment. |
|  | FRET\_expt | Categories that describe a fluorescence experiment. |
|  | EMR\_expt | Categories that describe an electron magnetic resonance experiment. |
|  | SAXS\_expt | Categories that describe a small angle X-ray scattering experiment. |
|  | computer | Categories that describe a computer. |
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| NMR\_parameters |  | The NMR\_parameters super group contains the category groups used to model NMR spectral parameters or theoretically calculated parameters like chemical shifts and links to supporting information. |
|  | chem\_shift\_reference | Categories that capture information about the compounds and parameters used to reference NMR chemical shifts. |
|  | assigned\_chemical\_shifts | Categories that capture assigned chemical shift values and links to the samples, sample conditions, NMR experiments, and other information about how the assigned chemical shifts were derived. |
|  | coupling\_constants | Categories that capture coupling constant values and links to the samples, sample conditions, NMR experiments, and other information about how the coupling constants were derived. |
|  | theoretical\_coupling\_constants | Categories that capture theoretical coupling constant values and links to the software, samples, sample conditions, NMR experiments, and other information about how the theoretical coupling constants were derived. |
|  | spectral\_peak\_list | Categories that capture the properties of NMR spectral peaks, spectral parameters, and links to the NMR experiments and other information regarding the data. |
|  | resonance\_linker | Categories that describe the linking of resonances to chemical spin systems and experimental results. |
|  | chem\_shift\_isotope\_effect | Categories that capture chemical shift isotope effect values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | chem\_shift\_perturbation | Categories that capture chemical shift deviations caused by molecular interactions and links to the samples, sample conditions, NMR experiments, and other information about how the deviation values were derived. |
|  | chem\_shift\_anisotropy | Categories that capture chemical shift anisotropy values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
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|  | theoretical\_chem\_shifts | Categories that capture theoretical chemical shift values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | chem\_shifts\_calc\_type | Categories that define the type of calculation used to generate a list of theoretical chemical shifts for a molecule. |
|  | RDCs | Categories that capture residual dipolar coupling values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | dipolar\_couplings | Categories that capture dipolar coupling values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | spectral\_density\_values | Categories that capture spectral density values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | other\_data\_types | Categories that capture the values for other kinds of data not modeled in specific category groups in the dictionary and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
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| kinetics |  | The kinetics super group contains the category groups that model a variety of kinetic values that can be derived from NMR spectral data. |
|  | chemical\_rates | Categories that capture chemical rate data and links to the samples, sample conditions, NMR experiments, and other information about how the data were collected and analyzed. |
|  | H\_exch\_rates | Categories that capture hydrogen exchange rate data and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | H\_exch\_protection\_factors | Categories that capture hydrogen exchange protection factor data and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | homonucl\_NOEs | Categories that capture homonuclear NOE values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | heteronucl\_NOEs | Categories that capture heteronuclear NOE values and links to the samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | theoretical\_heteronucl\_NOEs | Categories that capture theoretical heteronuclear NOE values and links to the software, samples, sample conditions, NMR experiments, and other information about how the values were derived. |
|  | heteronucl\_T1\_relaxation | Categories that capture heteronuclear T1 relaxation values and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | theoretical\_heteronucl\_T1\_relaxation | Categories that capture theoretical heteronuclear T1 relaxation values and links to the software, samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | heteronucl\_T1rho\_relaxation | Categories that capture heteronuclear T1rho relaxation values and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | heteronucl\_T2\_relaxation | Categories that capture heteronuclear T2 relaxation values and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | theoretical\_heteronucl\_T2\_relaxation | Categories that capture theoretical heteronuclear T2 relaxation values and links to the software, samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | auto\_relaxation | Categories that capture auto relaxation data and links to the samples, sample conditions, NMR experiments, and other information about how the data were collected and analyzed. |
|  | theoretical\_auto\_relaxation | Categories that capture theoretical auto relaxation data and links to the software, samples, sample conditions, NMR experiments, and other information about how the data were collected and analyzed. |
|  | dipole\_dipole\_relaxation | Categories that capture dipole-dipole relaxation values and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
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|  | dipole\_dipole\_cross\_correlations | Categories that capture dipole-dipole cross correlation data and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | theoretical\_dipole\_dipole\_cross\_correlations | Categories that capture theoretical dipole-dipole cross correlation data and links to the software, samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | dipole\_CSA\_cross\_correlations | Categories that capture dipole-CSA cross correlation data and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
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| thermodynamics |  | The thermodynamic super group contains the category groups that contain the thermodynamic data that can be derived from NMR spectral data. |
|  | order\_parameters | Categories that capture order parameter values and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | pH\_titration | Categories that capture the pKa or pHmid values derived from a pH titration experiment and links to the experimental details. |
|  | pH\_param\_list | Categories that capture the NMR spectral parameters derived from a pH titration experiment. |
|  | D\_H\_fractionation\_factors | Categories that capture deuterium-hydrogen fractionation factor values and links to the samples, sample conditions, NMR experiments, and other information about how the data were derived. |
|  | binding\_data | Categories that capture the binding data derived from a chemical binding experiment and links to the experimental details. |
|  | binding\_param\_list | Categories that capture the NMR spectral parameters derived from a chemical binding experiment. |
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| structure |  | The structure category super group captures atomic coordinates, constraints, statistical data, and other related information. |
|  | deduced\_secd\_struct\_features | Categories that capture secondary structure features deduced from experimental data, but not derived from a three-dimensional structure and links to the data used to deduce the secondary structure features. |
|  | deduced\_hydrogen\_bonds | Categories that capture hydrogen bonds information deduced from experimental data, but not derived from a three-dimensional structure and links to the data used to deduce the hydrogen bonds. |
|  | conformer\_statistics | Categories that capture statistics derived from the three-dimensional conformers calculated for a biomolecule. |
|  | constraint\_statistics | Categories that capture statistics derived from the constraints used to calculate the three-dimension conformers for a biomolecule and the constraint violations. |
|  | representative\_conformer | Categories that capture the atomic coordinates for a representative conformer of a biomolecular system and links to the experimental conditions and data used to derive the conformer. |
|  | conformer\_family\_coord\_set | Categories that capture the atomic coordinates for a family of conformers for a biomolecular system and links to the experimental conditions and data used to calculate the conformer family. |
|  | force\_constants | Categories that describe the values for the force constants used in calculating a family of conformers for a biomolecular system. |
|  | angular\_order\_parameters | Categories that capture a set of angular order parameters calculated from a family of conformers. |
|  | tertiary\_struct\_elements | Categories that describe the tertiary structure elements found in the conformers calculated for a biomolecular system. |
|  | structure\_annotation | Categories that describe annotations derived from PDB structure entries related to the BMRB entry and extracted from an external database or calculated by BMRB. |
|  | secondary\_structs | Categories that describe the secondary structure elements found in the conformers calculated for a biomolecular system. |
|  | bond\_annotation | Categories that capture annotations for the bonds found in the conformers calculated for a biomolecular system. |
|  | structure\_interactions | Categories that describe the interactions between molecules in a biomolecular system that have been found through the analysis of the calculated conformers. |
|  | other\_struct\_features | Categories that provide a means for describing other structure features not specifically defined in other category groups. |
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|  | tensor | Categories that describe tensors. |
|  | interatomic\_distance | Categories that describe a set of interatomic distances in a molecular assembly. |
|  | general\_distance\_constraints | Categories that capture the distance constraints in a simple table format used to calculate one or more conformers for a biomolecular system. |
|  | distance\_constraints | Categories that capture the distance constraints used to calculate one or more conformers for a biomolecular system. |
|  | floating\_chiral\_stereo\_assign | Categories that capture the floating chirality stereo assignments used in calculating the conformers for a biomolecular system. |
|  | torsion\_angle\_constraints | Categories that capture the torsion angle distance constraints used to calculate one or more conformers for a biomolecular system. |
|  | RDC\_constraints | Categories that capture the residual dipolar coupling constraints used to calculate one or more conformers for a biomolecular system. |
|  | J\_three\_bond\_constraints | Categories that capture the three bond scalar coupling constraints used to calculate one or more conformers for a biomolecular system. |
|  | CA\_CB\_chem\_shift\_constraints | Categories that capture the protein CA and CB chemical shift constraints used to calculate one or more conformers for a biomolecular system. |
|  | H\_chem\_shift\_constraints | Categories that capture the proton chemical shift constraints used to calculate one or more conformers for a biomolecular system. |
|  | Peak\_constraint\_list\_link | Categories that link spectral peaks in peak lists with the derived structural constraint. |
|  | SAXS\_constraints | Categories that capture the SAXS constraints used to calculate one or more conformers for a biomolecular system. |
|  | other\_constraints | Categories that capture values for other kinds of constraints not specifically defined in other category groups used to calculate one or more conformers for a biomolecular system. |
|  | org\_constr\_file\_comment | Categories that capture the comments extracted from one or more original constraint files. |
|  | MS\_MZ\_data | Categories that capture the MZ data from a mass spectrometry experiment. |
|  | MS\_chromatogram | Categories that capture the data from a MS chromatogram. |