NMR-STAR tags with unique definitions and data types

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| **Table S1.** Special tags and tags that are exceptions to the general rules. | |  |
| **Tag type** | **Usage** |  |
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| \_xxxx.Sf\_ID | An unique integer value that identifies save frames of the same category within an entry. For example, each ‘sample’ save frame is assigned a unique Sf\_ID value usually starting with the value ‘1’ and incrementing sequentially. These values are primarily for internal database management. |  |
| \_xxxx.Sf\_framecode | A string denoting the corresponding frame name. |  |
| \_xxxx.Sf\_category | The values for the Sf\_category tag define the type of object represented by the data in the save frame. |  |
| \_xxxx.xxx\_label | The values for these tags are STAR framecodes that are pointers to save frames within an NMR-STAR file. |  |
| \_xxxx.Comp\_ID | The values assigned to these tags are character strings that uniquely identify a chemical compound or chemical moiety. The values are often equivalent to the one-to-three letter codes used in the PDB ligand library. However, the values are not restricted to three letters and can be up to twelve characters in length. |  |
| \_xxxx.Atom\_ID | Atom\_ID values are effectively atom names. |  |
| \_xxxx.Entry\_ID | BMRB entry ID’s or accession codes may be either integer values, as for the biopolymer entries, or strings that are a combination of an alpha character(s) prefix and a string of numeric characters, as used for combined BMRB PDB entries, small molecule and natural product entries. |  |