Structure of a CIF Dictionary

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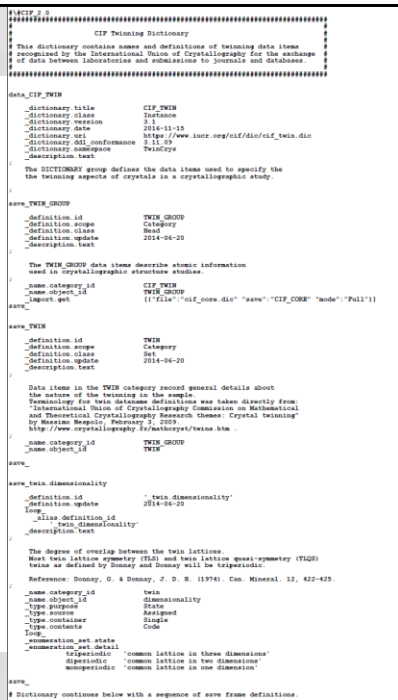
Dictionary definition languages

- DDL0
  - *ad hoc* notation developed for the initial CIF paper publication (1991)
- DDL1
  - formal standard for 'small-molecule' crystallography from 1995
- DDL2
  - developed for biological macromolecular applications from 2000
  - isomorphous to relational database (SQL) data description language
  - some materials in previous COMCIFS workshop (Hyderabad, 2017)
  - fully supported by wwPDB https://mmcif.wwpdb.org/
- DDLm
  - adopted by COMCIFS for new dictionaries in 2013
  - includes relational features developed in DDL2
  - supports methods for declaring and validating relationships between items

Dictionary layout (overview)

- By convention, dictionaries are laid out in an orderly fashion to facilitate human browsing and location of relevant information.
- As files conforming to the CIF format specification, they are equally valid to machine parsers if presented with different ordering and white space.
- A style guide is included in the workshop booklet.



Syntax header flag

Header comment, ignored by software

Overall dictionary information at the beginning of a data block.

Definition of the Head category for the dictionary ("TWIN_GROUP")

Definition of an ordinary category ("TWIN")

Definition of a data name ("_twin.dimensionality")

More data name and category definitions follow.

Dictionary layout

```
#\#CIF_2.0
##############################################################################
#                                                                            #
#                    CIF Twinning Dictionary                                 #
#                                                                            #
# This dictionary contains names and definitions of twinning data items      #
# recognized by the International Union of Crystallography for the exchange  #
# of data between laboratories and submissions to journals and databases.    #
#                                                                            #
##############################################################################
```

Syntax header flag

Header comment, ignored by software

- DDLm dictionaries are conventionally conformant to the CIF 2.0 syntax specification, *e.g.* to allow import statements of the type

```
_import.get      [{"file":"cif_core.dic" "save":"CIF_CORE" "mode":"Full"}]
```

- The header comment allows quick visual recognition by human readers.

Dictionary layout

```
data_CIF_TWIN

    _dictionary.title            CIF_TWIN
    _dictionary.class            Instance
    _dictionary.version          3.1
    _dictionary.date             2016-11-15
    _dictionary.uri              https://www.iucr.org/cif/dic/cif_twin.dic
    _dictionary.ddl_conformance  3.11.09
    _dictionary.namespace        TwinCrys
    _description.text
;
    This dictionary defines the data items used to specify the
    twinning aspects of crystals in a crystallographic study.
;
```

Overall dictionary information at the beginning of a data block

- All the definitions within a dictionary are contained in a single data block. The characteristics of the dictionary as a whole are reported at that data-block level.

Dictionary layout

```
save_TWIN_GROUP

    _definition.id               TWIN_GROUP
    _definition.scope            Category
    _definition.class            Head
    _definition.update           2014-06-20
    _description.text
;
     The TWIN_GROUP data items describe atomic information
     used in crystallographic structure studies.
;
    _name.category_id            CIF_TWIN
    _name.object_id              TWIN_GROUP
    _import.get                  [{"file":"cif_core.dic" "save":"CIF_CORE" "mode":"Full"}]

save_
```

Definition of the Head category for the dictionary ('TWIN_GROUP')

- The Head category establishes the root of the conceptual definitions tree. Importing another dictionary establishes the current dictionary as a proper superset of the imported one.

Dictionary layout

```
save_TWIN

    _definition.id                TWIN
    _definition.scope             Category
    _definition.class             Set
    _definition.update            2014-06-20
    _description.text
;
     Data items in the TWIN category record general details about
     the nature of the twinning in the sample.
     Terminology for twin dataname definitions was taken directly from:
     "International Union of Crystallography Commission on Mathematical
     and Theoretical Crystallography Research themes: Crystal twinning"
     by Massimo Nespolo, February 3, 2009.
     http://www.crystallography.fr/mathcryst/twins.htm
;
    _name.category_id             TWIN_GROUP
    _name.object_id               TWIN

save_
```

Definition of an ordinary category ('TWIN')

Dictionary layout

```
save_twin.dimensionality

    _definition.id                '_twin.dimensionality'
    _definition.update            2014-06-20
    loop_
      _alias.definition_id
          '_twin_dimensionality'
    _description.text
;
     The degree of overlap between the twin lattices.
     Most twin lattice symmetry (TLS) and twin lattice quasi-symmetry (TLQS)
     twins as defined by Donnay and Donnay will be triperiodic.

     Reference: Donnay, G. & Donnay, J. D. H. (1974). Can. Mineral. 12, 422-425.
;
    _name.category_id             twin
    _name.object_id               dimensionality
    _type.purpose                 State
    _type.source                  Assigned
    _type.container               Single
    _type.contents                Code
    loop_
    _enumeration_set.state
    _enumeration_set.detail
              triperiodic   'common lattice in three dimensions'
              diperiodic    'common lattice in two dimensions'
              monoperiodic  'common lattice in one dimension'

save_
```

Definition of a data name ('_twin.dimensionality')

More data name and category definitions follow. Conventionally, definitions of data names belonging to a category directly follow the category definition. Alphabetical ordering (within categories) is usual.

Dictionary layout

```
#==============================================================================
#  The dictionary's creation history.
#==============================================================================

     loop_
    _dictionary_audit.version
    _dictionary_audit.date
    _dictionary_audit.revision

      3.1    2016-11-16
;
   Initial CIF2 version created from STAR2 version provided by Syd Hall
   (J. Hester)
;
      3.1.1  2021-03-20
;
   Fixed a CIF2 syntax error.

   Removed the _description.text data item from
   the 'restr_angle.atom_site_label_1', 'restr_angle.atom_site_label_2'
   and 'restr_angle.atom_site_label_3' save frames since the same data
   item is already provided in the imported 'restr_label' save frame.

   (A. Vaitkus)
;
```

Revision history of the dictionary

By convention, this appears at the end of the dictionary.

Main pieces of information in a definition

- _description.text
- category_id, object_id
- _definition.id
- _name.linked_item_id

Optional information

- Instances of several additional attributes will appear in the examples to come.
- Full dictionary at https://www.iucr.org/resources/cif/ddl/ddlm (current release) and https://github.com/COMCIFS/cif_core/blob/master/ddl.dic (development version)
- The full DDLm dictionary (pretty formatted) is included in the workshop booklet.

Building a dictionary definition of a data item describing a physical quantity

```
Mean hydrostatic pressure at which intensities were measured.
```

*Begin with a textual description of the thing you want to define. Aim to be **concise**, yet **precise**.*

Building a dictionary definition of a data item describing a physical quantity

```
    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
```

Tag it with the appropriate DDLm attribute and enclose in suitable delimiters.

Building a dictionary definition of a data item describing a physical quantity

```
save_xxxx

    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;

save_
```

Each distinct definition is encapsulated in its own save frame. Each must have an identifier (initially 'xxxx' here) that is unique within the dictionary.

Building a dictionary definition of a data item describing a physical quantity

```
save_xxxx


     description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id               diffrn
    _name.object_id                 ambient_pressure


save_
```

How does this fit into the overall scheme of things? You will already have established an appropriate category; now assign a suitable tag.

Building a dictionary definition of a data item describing a physical quantity

```
save_xxxx

    _definition.id                  '_diffrn.ambient_pressure'


    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id               diffrn
    _name.object_id                 ambient_pressure


save_
```

These choices will suggest an obvious canonical form for the data name identifier.

Building a dictionary definition of a data item describing a physical quantity

```
save_xxxx

    _definition.id                  '_diffrn.ambient_pressure'


    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id               diffrn
    _name.object_id                 ambient_pressure




    _units.code                     kilopascals

save_
```

As this is the definition of a measurable physical quantity, we need to specify the physical units associated with any value.

Building a dictionary definition of a data item describing a physical quantity

```
save_diffrn.ambient_pressure

    _definition.id                  '_diffrn.ambient_pressure'

    _definition.update              2023-01-13
    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id               diffrn
    _name.object_id                 ambient_pressure




     units.code                     kilopascals

save_
```

We do some housekeeping (adopting the assigned data name as the save frame code and logging the change date) and we now have our minimal functioning definition.

Building a dictionary definition of a data item describing a physical quantity

```
save_diffrn.ambient_pressure

    _definition.id                  '_diffrn.ambient_pressure'

    _definition.update              2023-01-13
    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id               diffrn
    _name.object_id                 ambient_pressure



    _type.contents                  Real
    _enumeration.range              0.0:
    _units.code                     kilopascals

save_
```

But we can do more. For validation purposes, we can define the type and any sensible constraints on data values.

Building a dictionary definition of a data item describing a physical quantity

```
save_diffrn.ambient_pressure

    _definition.id                  '_diffrn.ambient_pressure'

    _definition.update              2023-01-13
    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id               diffrn
    _name.object_id                 ambient_pressure



    _type.container                 Single
    _type.contents                  Real
    _enumeration.range              0.0:
    _units.code                     kilopascals

save_
```

We also specify that data values are expected to be single (i.e. scalar, rather than matrix, list, array or table).

Building a dictionary definition of a data item describing a physical quantity

```
save_diffrn.ambient_pressure

    _definition.id                '_diffrn.ambient_pressure'

    _definition.update            2023-01-13
    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure
    _type.purpose                 Measurand
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _enumeration.range            0.0:
    _units.code                   kilopascals

save_
```

'Measurand' indicates that the value should have an associated standard uncertainty. _type.source is of use in integrity checking.

_type.source (*Code*)

The origin or source of the defined data item, indicating by what recording process it has been added to the domain instance.

Where no value is given, the assumed value is 'Assigned'.

The data value must be one of the following:

- Recorded
  - Data value (numerical or otherwise) was recorded by observation or measurement during the experimental collection of data. Data items of this type are considered primitive.
- Assigned
  - Data value (numerical or otherwise) was assigned as part of the data collection, analysis or modelling required for a specific domain instance. These assignments often represent a decision made that determines the course of the experiment (and therefore the data item may be deemed primitive) or a particular choice in the way the data was analysed (and therefore the data item may be considered non-primitive).
- Related
  - Data item was added based on a relationship to another data item. This state indicates that the item was used to record the SU value of a related measurand item or that the item was used in the construction of looped lists of data. In the latter case, it typically identifies an item whose unique values are used as the reference key for a loop category and/or an item which has values in common with those of another loop category and is considered a Link between these lists. Data items of this type include both primitive and non-primitive items.
- Derived
  - Data item was derived from other data items within the domain instance. Data items of this type are considered non-primitive.

Building a dictionary definition of a data item describing a physical quantity

```
save_diffrn.ambient_pressure

    _definition.id                '_diffrn.ambient_pressure'
    _alias.definition_id          '_diffrn_ambient_pressure'
    _definition.update            2023-01-13
    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure
    _type.purpose                 Measurand
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _enumeration.range            0.0:
    _units.code                   kilopascals

save_
```

Finally, alternative forms of the data name identifier may be listed. Usually this will identify equivalent definitions in legacy DDL1 dictionaries.

A dictionary definition of a data item describing a physical quantity

```
save_diffrn.ambient_pressure

    _definition.id                '_diffrn.ambient_pressure'
    _alias.definition_id          '_diffrn_ambient_pressure'
    _definition.update            2023-01-13
    _description.text
;
    Mean hydrostatic pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure
    _type.purpose                 Measurand
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _enumeration.range            0.0:
    _units.code                   kilopascals

save_
```

Definition of a data item describing the standard uncertainty associated with another item

```
save_diffrn.ambient_pressure_su
    _definition.id                '_diffrn.ambient_pressure_su'

    _definition.update             2021-03-03
    _description.text
;
    Standard uncertainty of the mean hydrostatic
    pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure_su

    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _units.code                   kilopascals
save_
```

Now we build up the definition for an associated standard uncertainty. The overall framework is the same as the previous case.

Definition of a data item describing the standard uncertainty associated with another item

```
save_diffrn.ambient_pressure_su
    _definition.id                '_diffrn.ambient_pressure_su'

    _definition.update             2021-03-03
    _description.text
;
    Standard uncertainty of the mean hydrostatic
    pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure_su

    _type.purpose                 SU
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _units.code                   kilopascals
save_
```

The most immediate distinction is identification of the value as a standard uncertainty.

_type.purpose (*Code*)

The primary purpose or function the defined data item serves in a dictionary or a specific data instance.

Where no value is given, the assumed value is 'Describe'.

The data value must be one of the following:

- Describe
  - Used to type items with values that are descriptive text intended for human interpretation.
- Key
  - Used to type an item with a value that is unique within the looped list of these items, and does not contain encoded information.
- Measurand
  - Used to type an item with a numerically estimated value that has been recorded by measurement or derivation. A data item definition for the standard uncertainty (SU) of this item must be provided in a separate definition with _type.purpose of 'SU'. The value of a measurand item should be accompanied by a value of its associated SU item, either: 1) integrated with the measurand value in a manner characteristic of the data format; or 2) as a separate, explicit value for the associated SU item. These alternatives are semantically equivalent.
- SU
  - Used to type an item with a numerical value that is the standard uncertainty of another data item. The definition of an SU item must include the attribute '_name.linked_item_id' which explicitly identifies the associated measurand item. SU values must be non-negative.
- *etc. …*

Definition of a data item describing the standard uncertainty associated with another item

```
save_diffrn.ambient_pressure_su
    _definition.id                '_diffrn.ambient_pressure_su'
    _definition.update             2021-03-03
    _description.text
;
    Standard uncertainty of the mean hydrostatic
    pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure_su
    _name.linked_item_id          '_diffrn.ambient_pressure'
    _type.purpose                 SU
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _units.code                   kilopascals
save_
```

It is essential to link this item to the item for which it records the standard uncertainty.

Definition of a data item describing the standard uncertainty associated with another item

```
save_diffrn.ambient_pressure_su
    _definition.id                '_diffrn.ambient_pressure_su'
    loop_
      _alias.definition_id
         '_diffrn_ambient_pressure_su'
         '_diffrn.ambient_pressure_esd'
    _definition.update             2021-03-03
    _description.text
;
    Standard uncertainty of the mean hydrostatic
    pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure_su
    _name.linked_item_id         '_diffrn.ambient_pressure'
    _type.purpose                 SU
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _units.code                   kilopascals
save_
```

And in this case there are also legacy aliases (the _esd one reflecting practice in MX).

Definition of a data item describing the standard uncertainty associated with another item

```
save_diffrn.ambient_pressure_su
    _definition.id                '_diffrn.ambient_pressure_su'
    loop_
      _alias.definition_id
         '_diffrn_ambient_pressure_su'
         '_diffrn.ambient_pressure_esd'
    _definition.update             2021-03-03
    _description.text
;
    Standard uncertainty of the mean hydrostatic
    pressure at which intensities were measured.
;
    _name.category_id             diffrn
    _name.object_id               ambient_pressure_su
    _name.linked_item_id         '_diffrn.ambient_pressure'
    _type.purpose                 SU
    _type.source                  Recorded
    _type.container               Single
    _type.contents                Real
    _units.code                   kilopascals
save_
```

Two ways to present a standard uncertainty

```
_diffrn.ambient_pressure          100.5(2)
```

```
_diffrn.ambient_pressure          100.5
_diffrn.ambient_pressure_su       0.2
```

Use of an _su data item is not mandatory in a data file; the value can be appended to the primary data value in parentheses.

A data item that can take only one of a discrete set of allowed values

```
save_pd_spec.mount_mode
    _definition.id                '_pd_spec.mount_mode'
    _alias.definition_id          '_pd_spec_mount_mode'
    _definition.update             2014-06-20
    _description.text
;
    A code describing the beam path through
    the specimen.
;
    _name.category_id              pd_spec
    _name.object_id                mount_mode




save_
```

We will now look at a case where the value of a data item may take only one of a fixed set of values.

A data item that can take only one of a discrete set of allowed values

```
save_pd_spec.mount_mode
    _definition.id                '_pd_spec.mount_mode'
    _alias.definition_id          '_pd_spec_mount_mode'
    _definition.update             2014-06-20
    _description.text
;
    A code describing the beam path through
    the specimen.
;
    _name.category_id              pd_spec
    _name.object_id                mount_mode


    _type.container                Single
    _type.contents                 Code




save_
```

The type is set as 'code'

A data item that can take only one of a discrete set of allowed values

```
save_pd_spec.mount_mode
    _definition.id                '_pd_spec.mount_mode'
    _alias.definition_id          '_pd_spec_mount_mode'
    _definition.update             2014-06-20
    _description.text
;
    A code describing the beam path through
    the specimen.
;
    _name.category_id              pd_spec
    _name.object_id                mount_mode
    _type.purpose                  Encode
    _type.source                   Assigned
    _type.container                Single
    _type.contents                 Code




save_
```

… and the purpose as 'Encode'.

A data item that can take only one of a discrete set of allowed values

```
save_pd_spec.mount_mode
    _definition.id                '_pd_spec.mount_mode'
    _alias.definition_id          '_pd_spec_mount_mode'
    _definition.update             2014-06-20
    _description.text
;
    A code describing the beam path through
    the specimen.
;
    _name.category_id              pd_spec
    _name.object_id                mount_mode
    _type.purpose                  Encode
    _type.source                   Assigned
    _type.container                Single
    _type.contents                 Code
    loop_
      _enumeration_set.state
        reflection
        transmission
save_
```

The allowed values are then looped. If the meaning is not clear, the loop may also contain an explanatory `_enumeration_set.detail`

A data item that can take only one of a discrete set of allowed values

```
save_pd_spec.mount_mode
    _definition.id                '_pd_spec.mount_mode'
    _alias.definition_id          '_pd_spec_mount_mode'
    _definition.update             2014-06-20
    _description.text
;
    A code describing the beam path through
    the specimen.
;
    _name.category_id              pd_spec
    _name.object_id                mount_mode
    _type.purpose                  Encode
    _type.source                   Assigned
    _type.container                Single
    _type.contents                 Code
    loop_
      _enumeration_set.state
        reflection
        transmission
save_
```

Definition of a category

```
save_ATOM_SITE

    _definition.update              2023-02-03
    _description.text
;
    The CATEGORY of data items used to describe atom site information
    used in crystallographic structure studies.
;

save_
```

The definition of an entire category begins with the same framework.

Definition of a category

```
save_ATOM_SITE

    _definition.id                  ATOM_SITE
    _definition.scope               Category

    _definition.update              2023-02-03
    _description.text
;
    The CATEGORY of data items used to describe atom site information
    used in crystallographic structure studies.
;
    _name.category_id               ATOM
    _name.object_id                 ATOM_SITE

save_
```

The category itself also belongs to a category. The root of the category tree is known as the Head category.

Definition of a category

```
save_ATOM_SITE

    _definition.id                ATOM_SITE
    _definition.scope             Category
    _definition.class             Loop
    _definition.update            2023-02-03
    _description.text
;
    The CATEGORY of data items used to describe atom site information
    used in crystallographic structure studies.
;
    _name.category_id             ATOM
    _name.object_id               ATOM_SITE


save_
```

Most categories describe tabulated data that are looped. But in some cases, only one instance of each item is expected; there, `_definition.class` is 'Set'

Definition of a category

```
save_ATOM_SITE

    _definition.id                ATOM_SITE
    _definition.scope             Category
    _definition.class             Loop
    _definition.update            2023-02-03
    _description.text
;
    The CATEGORY of data items used to describe atom site information
    used in crystallographic structure studies.
;
    _name.category_id             ATOM
    _name.object_id               ATOM_SITE
    _category_key.name            '_atom_site.label'

save_
```

Essential for referential integrity of the category is the declaration of its key value(s).

Definition of a category

```
save_ATOM_SITE

    _definition.id                  ATOM_SITE
    _definition.scope               Category
    _definition.class               Loop
    _definition.update              2023-02-03
    _description.text
;
    The CATEGORY of data items used to describe atom site information
    used in crystallographic structure studies.
;
    _name.category_id               ATOM
    _name.object_id                 ATOM_SITE
    _category_key.name              '_atom_site.label'

save_
```


Example of a category (relational table)

```
loop_
    _description_example.case
    _description_example.detail
;
        loop_
          _atom_site.label
          _atom_site.type_symbol
          _atom_site.fract_x
          _atom_site.fract_y
          _atom_site.fract_z
          _atom_site.occupancy
          _atom_site.disorder_assembly
          _atom_site.disorder_group
           Cu1 Cu 0.78443(2) 0.88297(4) 0.37825(2)  1       . .
           Co1 Co 0.77504(2) 0.66957(4) 0.54249(2)  0.78(3) A 1
           Mn1 Mn 0.77504(2) 0.66957(4) 0.54249(2)  0.22(3) A 2
           O1   O 0.85532(9) 0.95747(19) 0.28965(9) 1       . .
           O2   O 0.84868(9) 0.94662(19) 0.14953(8) 1       . .
           # ...
;
;
        An example of a compositional disorder description. Disorder assembly
        'A' describes a site that is simultaneously occupied by Co and Mn
        atoms which are assigned to disorder group '1' and disorder group '2'
        respectively.

        The example was created based on data from:
            Li, Ang et al. (2021). Dalton Transactions, 50(2), 681-688.
;
```

*We will examine this example in a moment. What we are showing here is how an example is actually presented **within** the dictionary.*

Example of a category (relational table)

```
loop_
        _atom_site.label
        _atom_site.type_symbol
        _atom_site.fract_x
        _atom_site.fract_y
        _atom_site.fract_z
        _atom_site.occupancy
        _atom_site.disorder_assembly
        _atom_site.disorder_group
        Cu1 Cu 0.78443(2) 0.88297(4) 0.37825(2)  1        . .
        Co1 Co 0.77504(2) 0.66957(4) 0.54249(2)  0.78(3) A 1
        Mn1 Mn 0.77504(2) 0.66957(4) 0.54249(2)  0.22(3) A 2
        O1   O 0.85532(9) 0.95747(19) 0.28965(9) 1        . .
        O2   O 0.84868(9) 0.94662(19) 0.14953(8) 1        . .
        # ...
```

And in the example itself, we see how the looping is set up; the category key is highlighted.

Example of a category (relational table)

```
loop_ _atom_site.label _atom_site.type_symbol
      _atom_site.fract_x _atom_site.fract_y _atom_site.fract_z
      _atom_site.occupancy _atom_site.disorder_assembly
      _atom_site.disorder_group Cu1 Cu 0.78443(2) 0.88297(4)
0.37825(2)  1 . . Co1 Co 0.77504(2) 0.66957(4) 0.54249(2)
0.78(3) A 1 Mn1 Mn 0.77504(2) 0.66957(4) 0.54249(2) 0.22(3)
A 2 O1 O 0.85532(9) 0.95747(19) 0.28965(9) 1 . . O2 O 0.84868(9)
0.94662(19) 0.14953(8) 1 . .
# ...
```

And this is just to emphasise that a neat layout is not essential. This example is completely legitimate.

A child category: can be presented as a standalone loop structure or folded into its parent category

```
save_ATOM_SITE_ANISO

    _definition.id                  ATOM_SITE_ANISO
    _definition.scope               Category
    _definition.class               Loop
    _definition.update              2023-01-16
    _description.text
;
    The CATEGORY of data items used to describe the anisotropic atomic
    displacement parameters of the atomic sites in a crystal structure.
;
    _name.category_id               ATOM_SITE
    _name.object_id                 ATOM_SITE_ANISO
    _category_key.name              '_atom_site_aniso.label'

save_
```

Sparse subsets of some tables are traditionally represented in separate tables. Category parent–child relationships facilitate this.

Category and child category

```
loop_
  _atom_site_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_thermal_displace_type
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
    Fe(1) 0.1394(1) 0.20486(7) 0.1593(2) Uani
       0.042(1) 0.042(1) 0.045(1) 0.0117(7) -0.0096(7) -0.0063(7)
    S(1) 0.2719(2) 0.2828(1) 0.0844(3) Uani
       0.049(2) 0.050(2) 0.043(2) 0.009(1) -0.005(1) -0.004(1)
    F(1) 0.4648(7) 0.1355(4) 0.0836(8) Uani
       0.147(8) 0.142(7) 0.098(6) 0.095(6) -0.008(6) -0.018(5)
    F(2) 0.5636(8) 0.0989(4) 0.251(1) Uani
       0.23(1) 0.122(7) 0.119(7) 0.113(8) -0.016(7) 0.008(6)
    F(3) 0.6251(8) 0.1729(5) 0.124(1) Uani
       0.15(1) 0.19(1) 0.29(1) 0.025(8) 0.14(1) -0.02(1)
    F(4) 0.0967(6) 0.4364(4) 0.0241(9) Uani
       0.132(7) 0.072(5) 0.148(7) 0.042(5) -0.066(6) -0.013(5)
    F(5) 0.0740(6) 0.5104(4) 0.176(1) Uani
       0.102(7) 0.125(7) 0.18(1) 0.058(6) 0.028(6) 0.028(6)
    F(6) 0.1806(6) 0.5374(4) 0.038(1) Uani
       0.141(7) 0.080(6) 0.135(7) 0.015(5) 0.004(6) 0.042(5)
```

```
loop_
  _atom_site.label
  _atom_site.fract_x
  _atom_site.fract_y
  _atom_site.fract_z
  _atom_site.thermal_displace_type
    Fe(1) 0.1394(1) 0.20486(7) 0.1593(2) Uani
    S(1) 0.2719(2) 0.2828(1) 0.0844(3) Uani
    F(1) 0.4648(7) 0.1355(4) 0.0836(8) Uani
    F(2) 0.5636(8) 0.0989(4) 0.251(1) Uani
    F(3) 0.6251(8) 0.1729(5) 0.124(1) Uani
    F(4) 0.0967(6) 0.4364(4) 0.0241(9) Uani
    F(5) 0.0740(6) 0.5104(4) 0.176(1) Uani
    F(6) 0.1806(6) 0.5374(4) 0.038(1) Uani

loop_
  _atom_site_aniso.label
  _atom_site_aniso.U_11
  _atom_site_aniso.U_22
  _atom_site_aniso.U_33
  _atom_site_aniso.U_12
  _atom_site_aniso.U_13
  _atom_site_aniso.U_23
    Fe(1) 0.042(1) 0.042(1) 0.045(1) 0.0117(7) -0.0096(7) -0.0063(7)
    S(1) 0.049(2) 0.050(2) 0.043(2) 0.009(1) -0.005(1) -0.004(1)
    F(1) 0.147(8) 0.142(7) 0.098(6) 0.095(6) -0.008(6) -0.018(5)
    F(2) 0.23(1) 0.122(7) 0.119(7) 0.113(8) -0.016(7) 0.008(6)
    F(3) 0.15(1) 0.19(1) 0.29(1) 0.025(8) 0.14(1) -0.02(1)
    F(4) 0.132(7) 0.072(5) 0.148(7) 0.042(5) -0.066(6) -0.013(5)
    F(5) 0.102(7) 0.125(7) 0.18(1) 0.058(6) 0.028(6) 0.028(6)
    F(6) 0.141(7) 0.080(6) 0.135(7) 0.015(5) 0.004(6) 0.042(5)
```

Example of dREL method

```
save_exptl_crystal.density_diffrn

    _definition.id                '_exptl_crystal.density_diffrn'
    _alias.definition_id          '_exptl_crystal_density_diffrn'
    _definition.update            2012-11-22
    _description.text
;
    Crystal density calculated from crystal unit cell and atomic content.
;
    _name.category_id             exptl_crystal
    _name.object_id               density_diffrn
    _type.purpose                 Measurand
    _type.source                  Derived
    _type.container               Single
    _type.contents                Real
    _enumeration.range            0.0:
    _units.code                   megagrams_per_metre_cubed
    _method.purpose               Evaluation
    _method.expression
;
    _exptl_crystal.density_diffrn = 1.6605 * _cell.atomic_mass / _cell.volume
;

save_
```

A (relatively) simple example of an evaluation method. If the crystal density does not appear in the data file, but other relevant information is present, it can be evaluated.

Example of dREL method

```
save_atom_type.number_in_cell

    _definition.id                '_atom_type.number_in_cell'
    _description.text
;   Total number of atoms of this atom type in the unit cell.
;
    _type.purpose                 Number
    _type.source                  Derived
    _units.code                   none
    _method.purpose               Evaluation
    _method.expression
;
    With t as atom_type
    cnt =  0.

    Loop a  as  atom_site  {
       if ( a.type_symbol == t.symbol ) {

          cnt +=  a.occupancy * a.site_symmetry_multiplicity
    }  }
    _atom_type.number_in_cell =  cnt
;

save_
```

This more complex example demonstrates dREL programming constructs and the ability to combine values from different categories.

(Some elements of the definition save frame omitted for space reasons.)