

## 3. CIF DATA DEFINITION AND CLASSIFICATION

Example 3.1.5.3. A simple definition of a data item describing a physical quantity.

```
data_diffn_ambient_temperature
  _name          '_diffn_ambient_temperature'
  _category      diffn
  _type          numb
  _type_conditions esd
  _enumeration_range 0.0:
  _units         K
  _units_detail   kelvin
  _definition
;   The mean temperature in kelvins at which the
    intensities were measured.
;
```

specified (0.0:) indicates that it may be any non-negative real number. The physical units of the quantity are also indicated.

The `_definition` attribute is a concise human-readable documentation of the meaning associated with the data name.

Example 3.1.5.4 is taken from the powder dictionary and illustrates a data item that can have only one of a limited set of values. This data item indicates the geometry of the experiment. The associated data value is of type *char* and may legally take only one of the two possible values listed.

## 3.1.5.4.2. Looped data

Many of the attributes of looped data items, such as their physical units or valid numerical values, may be defined in exactly the same way as for non-looped data. However, more care needs to be taken to describe the relationships between different looped data items.

Consider the following example listing of some three-dimensional atom-site coordinates and displacement parameters.

```
loop_
  _atom_site_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_thermal_displace_type
O1 .4154(4) .56990(10) .3026000 .0600(10) Uani
C2 .5630(5) .5087(2) .32460(10) .060(2) Uani
C3 .5350(5) .4920(2) .39970(10) .0480(10) Uani
N4 .3570(3) .55580(10) .4167000 .0390(10) Uani
C5 .3000(5) .6122(2) .35810(10) .0450(10) 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
O1 .071(1) .076(1) .0342(9) .008(1) .0051(9) -.0030(9)
C2 .060(2) .072(2) .047(1) .002(2) .013(1) -.009(1)
C3 .038(1) .060(2) .044(1) .007(1) .001(1) -.005(1)
N4 .037(1) .048(1) .0325(9) .0025(9) .0011(9) -.0011(9)
C5 .043(1) .060(1) .032(1) .001(1) -.001(1) .001(1)
```

```
loop_
  _geom_bond_atom_site_label_1
  _geom_bond_atom_site_label_2
  _geom_bond_distance
O1 C2 1.342(4)
O1 C5 1.439(3)
C2 C3 1.512(4)
C2 O21 1.199(4)
```

These loops, or tables of values, are properties of atom sites, each identified by a label such as O1. The definition of a data name such as `_atom_site_U_iso_or_equiv` expresses this by using the `DDL1_list_reference` attribute (Example 3.1.5.5).

Example 3.1.5.4. A data item that can take only one of a discrete set of allowed values.

```
data_pd_spec_mount_mode
  _name          '_pd_spec_mount_mode'
  _category      pd_spec
  _type          char
  _loop_enumeration reflection
                    transmission
  _definition
;   A code describing the beam path through
    the specimen.
;
```

Example 3.1.5.5. Definition relating a looped data item to the item used to identify a 'loop packet', or row of entries in a table.

```
data_atom_site_U_iso_or_equiv
  _name          '_atom_site_U_iso_or_equiv'
  _category      atom_site
  _type          numb
  _type_conditions esd
  _list          yes
  _list_reference '_atom_site_label'
```

Example 3.1.5.6. Definition of a mandatory item within a loop.

```
data_atom_site_label
  _name          '_atom_site_label'
  _category      atom_site
  _type          char
  _list          yes
  _list_mandatory yes
  loop_list_link_child
    '_atom_site_aniso_label'
    '_geom_bond_atom_site_label_1'
    '_geom_bond_atom_site_label_2'
```

For an entry in the table to make sense, the site identifier must be present, so the definition for `_atom_site_label` declares it a mandatory item within its list (Example 3.1.5.6).

It is common for an atom-site identifier to be used in several related tabulations in a particular crystal structure description, and in a CIF description this means that it may occur in several different looped lists. The dictionary definition gives a formal account of this by listing the data names in other looped lists which are just different manifestations of this same item. This is done using the `_list_link_child` attribute, which identifies the data names to which the one being currently defined is 'parent'. In Example 3.1.5.6 (which is a subset of the full list in the core dictionary), `_atom_site_aniso_label`, `_geom_bond_atom_site_label_1` and `_geom_bond_atom_site_label_2` are identified as children of `_atom_site_label`.

It can be seen immediately that `_atom_site_aniso_label` is the atom-site identification label appearing in the second table in the example listing above, and the `_geom_bond` items are clearly atom-site labels in a table of bonding properties between specified sites. There is, however, a difference between the two secondary tables: the bond-properties table is described by data items in the `GEOM_BOND` category, but the table of anisotropic displacement parameters includes data names that have the same `_category` attribute as the coordinate data items, namely `ATOM_SITE`. The latter is an example of multiple lists or tables belonging to the same category, a feature permitted only in DDL1-based data files.

## 3.1.5.4.3. Units

The physical units in which a quantitative data item must be expressed are identified by the DDL1 attributes `_units` and