2.5. SPECIFICATION OF THE CORE CIF DICTIONARY DEFINITION LANGUAGE (DDL1)

```
###############
## ATOM_SITE ##
###############
data_atom_site_[]
    _name                     '_atom_site_[]'
    _category                 category_overview
    _type                     null
    loop_  _example
           _example_detail
# - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - based on data set TOZ of Willis,
    Beckwith & Tozer [Acta Cryst. (1991), C47,
    2276-2277].
;
;   loop_
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_adp_type
    _atom_site_calc_flag
    _atom_site_calc_attached_atom
O1   .4154(4)  .5699(1)  .3026(0)  .060(1)  Uani  ? ?
C2   .5630(5)  .5087(2)  .3246(1)  .060(2)  Uani  ? ?
C3   .5350(5)  .4920(2)  .3997(1)  .048(1)  Uani  ? ?
N4   .3570(3)  .5558(1)  .4167(0)  .039(1)  Uani  ? ?
# - - - - data truncated for brevity - - - -
H321C  .04(1)   .318(3)   .320(2)   .14000   Uiso  ? ?
H322A  .25(1)   .272(4)   .475(3)   .19000   Uiso  ? ?
H322B  .34976   .22118    .40954    .19000   Uiso
                                             calc C322
;
# - - - - - - - - - - - - - - - - - - - - - - -
;   Example 2 - based on data set DPTD of Yamin,
    Suwandi, Fun, Sivakumar & bin Shawkataly
    [Acta Cryst. (1996), C52, 951-953].
;
;   loop_
    _atom_site_label
    _atom_site_chemical_conn_number
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
S1  1  0.74799(9)  -0.12482(11) 0.27574(9) 0.0742(3)
S2  2  1.08535(10)  0.16131(9)  0.34061(9) 0.0741(3)
N1  3  1.0650(2)   -0.1390(2)   0.2918(2)  0.0500(5)
C1  4  0.9619(3)   -0.0522(3)   0.3009(2)  0.0509(6)
# - - - - data truncated for brevity - - - -
;
    _definition
;   Data items in the ATOM_SITE category record
    details about the atom sites in a crystal
    structure, such as the positional
    coordinates, atomic displacement parameters,
    and magnetic moments and directions.
;
```

Fig. 2.5.5.5. DDL1 overview of a category of items.

2.5.5.9. Definition example 9: enumeration states

The last example, in Fig. 2.5.5.9, shows the definition of an item whose value is restricted to a predictable set of values known as enumeration states. The attributes `_enumeration` and `_enumeration_detail` are used to specify which enumeration states are permitted for the defined data item. Only one of these states may appear as the value for the defined item in a CIF. The attribute `_enumeration_default` specifies the state value that is used if an item is not instantiated.

```
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_angle_atom_site_label_1'
                '_geom_angle_atom_site_label_2'
                '_geom_angle_atom_site_label_3'
                '_geom_bond_atom_site_label_1'
                '_geom_bond_atom_site_label_2'

    loop_  _example    C12     Ca3g28      Fe3+17
                       H*251  boron2a  C_a_phe_83_a_0
                       Zn_Zn_301_A_0
    _definition
;   The _atom_site_label is a unique identifier for
    a particular site in the crystal.
;
```

Fig. 2.5.5.6. DDL1 definition of a 'mandatory' data item.

```
data_atom_site_aniso_label
    _name                     '_atom_site_aniso_label'
    _category                 atom_site
    _type                     char
    _list                     yes
    _list_link_parent     '_atom_site_label'
    _definition
;   Anisotropic atomic displacement parameters are
    usually looped in a separate list. If this is the
    case, this code must match the _atom_site_label
    of the associated atom in the atom coordinate
    list and conform with the same rules described
    in _atom_site_label.
;
```

Fig. 2.5.5.7. DDL1 definition of a 'parent' data item.

```
data_atom_site_aniso_U_
    loop_  _name              '_atom_site_aniso_U_11'
                              '_atom_site_aniso_U_12'
                              '_atom_site_aniso_U_13'
                              '_atom_site_aniso_U_22'
                              '_atom_site_aniso_U_23'
                              '_atom_site_aniso_U_33'
    _category                 atom_site
    _type                     numb
    _type_conditions          su
    _list                     yes
    _list_reference       '_atom_site_aniso_label'
    _related_item         '_atom_site_aniso_B_'
    _related_function         conversion
    _units                    A^2^
    _units_detail         'angstroms squared'
    _definition
;   These are the standard anisotropic atomic
    displacement components in angstroms squared.
;
```

Fig. 2.5.5.8. DDL1 definition showing 'related' data items.

2.5.6. DDL1 attribute descriptions

This section provides an overview of the different attributes that make up the core data dictionary language DDL1. A more detailed description of attributes is given in the DDL1 dictionary in Chapter 4.9. In this dictionary the attributes are used to define themselves!