3. CIF DATA DEFINITION AND CLASSIFICATION

3.6.7.6. Crystal symmetry

The categories describing symmetry are as follows:

SYMMETRY group

    SYMMETRY

    SYMMETRY_EQUIV

    SPACE_GROUP

    SPACE_GROUP_SYMOP

Data items in the SYMMETRY category are used to give details about the crystallographic symmetry. The equivalent positions for the space group are listed using data items in the SYMMETRY_EQUIV category. These categories are used in the same way in the core CIF and mmCIF dictionaries, and Section 3.2.4.4 can be consulted for details.

The current version of the mmCIF dictionary includes the SPACE_GROUP categories that were derived from the symmetry CIF dictionary (Chapter 3.8) and included in version 2.3 of the core CIF dictionary. At the time of writing, macromolecular applications have not yet begun to make use of these new categories.

Data items in these categories are as follows:

(*a*) SYMMETRY

● `_symmetry.entry_id`
    → `_entry.id`
  `_symmetry.cell_setting`
  `_symmetry.Int_Tables_number`
  `_symmetry.space_group_name_Hall`
  `_symmetry.space_group_name_H-M`

(*b*) SYMMETRY_EQUIV

● `_symmetry_equiv.id` (∼ `_symmetry_equiv_pos_site_id`)
  `_symmetry_equiv.pos_as_xyz`

(*c*) SPACE_GROUP

● `_space_group.id`
  `_space_group.crystal_system`
  `_space_group.IT_number`
  `_space_group.name_H-M_alt`
  `_space_group.name_Hall`

(*d*) SPACE_GROUP_SYMOP

● `_space_group_symop.id`
  `_space_group_symop.operation_xyz`
  `_space_group_symop.sg_id`

The bullet (●) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics have aliases in the core CIF dictionary formed by changing the full stop (.) to an underscore (_) except where indicated by the ∼ symbol.

The data item `_symmetry.entry_id` has been added to the SYMMETRY category to provide the formal category key required by the DDL2 data model.

3.6.7.7. Bond-valence information

The categories describing bond valences are as follows:

VALENCE group

    VALENCE_PARAM

    VALENCE_REF

These categories were introduced into version 2.2 of the core CIF dictionary to provide the information about bond valences required in inorganic crystallography. They appear in the mmCIF dictionary only for full compatibility with the core dictionary.

Data items in these categories are as follows:

(*a*) VALENCE_PARAM

● `_valence_param.atom_1`
● `_valence_param.atom_1_valence`
● `_valence_param.atom_2`
● `_valence_param.atom_2_valence`
  `_valence_param.B`
  `_valence_param.details`
  `_valence_param.id`

`_valence_param.ref_id`
    → `_valence_ref.id`
`_valence_param.Ro`

(*b*) VALENCE_REF

● `_valence_ref.id`
  `_valence_ref.reference`

The bullet (●) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics have aliases in the core CIF dictionary formed by changing the full stop (.) to an underscore (_).

Information about the use of these data items in the core CIF dictionary is given in Section 3.2.4.5.

3.6.8. Publication

The results of the determination of the crystal structure of a biological macromolecule might be published in an academic journal and/or deposited in a structural database. The data items in the core CIF dictionary cover most of the requirements for constructing an article for publication from an mmCIF and the many well defined data fields in mmCIF allow an extensively annotated record of the structure to be deposited in a database. However, the formalism of two of the core CIF categories for publication did not fit the relational database model of mmCIF, so new categories were required. The core CIF category COMPUTING, which is used to list the programs used to determine the structure, is replaced by the mmCIF category SOFTWARE, and the core CIF category DATABASE, which is used to identify the records associated with the structure in various databases, is replaced by the mmCIF category DATABASE_2.

The category groups discussed here are: the CITATION group, which is used to give citations to the literature (Section 3.6.8.1); the COMPUTING group, which is used to cite software (Section 3.6.8.2); the DATABASE group for citing related database entries (Section 3.6.8.3), which includes a group of categories used to ensure compatibility with specific database records in the Protein Data Bank (Section 3.6.8.3.2); journal administration categories that might be used by a publisher (Section 3.6.8.4.1); and the PUBL family of categories used to store the text of an article for publication (Section 3.6.8.4.2).

3.6.8.1. Literature citations

The categories describing literature citations are as follows:

CITATION group

    CITATION

    CITATION_AUTHOR

    CITATION_EDITOR

Data items in these categories are as follows:

(*a*) CITATION

● `_citation.id`
  `_citation.abstract`
  `_citation.abstract_id_CAS`
  `_citation.book_id_ISBN`
  `_citation.book_publisher`
  `_citation.book_publisher_city`
  `_citation.book_title`
  `_citation.coordinate_linkage`
  `_citation.country`
  `_citation.database_id_CSD`
  `_citation.database_id_Medline`
  `_citation.journal_abbrev`
  `_citation.journal_full`
  `_citation.journal_id_ASTM`
  `_citation.journal_id_CSD`
  `_citation.journal_id_ISSN`
  `_citation.journal_issue`
  `_citation.journal_volume`
  `_citation.language`
  `_citation.page_first`

190