assigned. The addition of algorithmic methods in future versions of CIF dictionaries will allow many of the symmetry items to be calculated as needed from expressions included in the dictionary as long as a space-group generator, such as the Hall symbol, is present in the CIF.

The symmetry CIF dictionary is written in DDL2 (Chapter 2.6) as this allows the relationships between the items to be given explicitly. Version 1.0 of the dictionary contains CIF definitions for all the basic symmetry items needed to describe a three-dimensional space group as described in more detail in Section 3.8.3. Some of these items have been incorporated in the core CIF dictionary, in which they have been converted to DDL1 (Chapter 2.5) to match the dictionary definition language of the core CIF dictionary. While the items in the symmetry CIF dictionary are designed in part to replace those in the symmetry category of the original core CIF dictionary, they are defined in a way that allows a CIF to include descriptions of several space groups in several settings. A single CIF could, in principle, include the symmetry operations and Wyckoff positions of all possible settings of the 230 space groups.

3.8.3. Arrangement of the dictionary

The three categories in version 1.0 of the symmetry CIF dictionary all lie within the SPACE_GROUP category group and are classified among the category groups defining the structural model listed in Section 3.1.10. (For convenience, in Chapters 3.2 and 3.4 the **_space_group_*** items introduced from the symmetry dictionary to the core and modulated structures dictionaries are discussed within an informal DDL1 SYMMETRY category group.)

The categories in the symmetry CIF dictionary are:

SPACE_GROUP
SPACE_GROUP_SYMOP
SPACE_GROUP_WYCKOFF

The first describes the properties of the space group as a whole, the second describes the properties of the symmetry operations and the third describes the properties of the special positions. The three categories are linked by a space-group identifier which allows items looped in the last two categories to be related back to one of the space groups defined in the first.

Data items in these categories are as follows:

(*a*) SPACE_GROUP

- ***_space_group.id***
  _space_group.Bravais_type
  _space_group.centring_type
  _space_group.crystal_system
  _space_group.Laue_class

  _space_group.IT_number
  _space_group.name_Hall
  _space_group.name_H-M_alt
  _space_group.name_H-M_alt_description
  _space_group.name_H-M_full
  _space_group.name_H-M_ref
  _space_group.name_Schoenflies
  _space_group.Patterson_name_H-M
  _space_group.point_group_H-M
  _space_group.reference_setting
  _space_group.transform_Pp_abc
  _space_group.transform_Qq_xyz

(*b*) SPACE_GROUP_SYMOP

- ***_space_group_symop.id***
  _space_group_symop.generator_xyz
  _space_group_symop.operation_description
  _space_group_symop.operation_xyz
  _space_group_symop.sg_id
  → _space_group.id

(*c*) SPACE_GROUP_WYCKOFF

- **_space_group_Wyckoff.id**
  _space_group_Wyckoff.coords_xyz
  _space_group_Wyckoff.letter
  _space_group_Wyckoff.multiplicity
  _space_group_Wyckoff.sg_id
  → _space_group.id
  _space_group_Wyckoff.site_symmetry

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics are also found in the core CIF dictionary.

The information contained in the SPACE_GROUP category relates to the properties of the space group as a whole. Three different kinds of properties are defined here.

Firstly, the names (or symbols) used to describe the space group are defined. As mentioned above, these divide themselves into ones that identify the space group without specifying any particular setting, and ones that can be used to generate the symmetry operations and therefore also specify the setting. Because of the ambiguities involved in the Hermann–Mauguin symbol, three different versions are defined with different degrees of rigour. **_space_group.name_H-M_ref** may only include the Hermann–Mauguin symbol of the reference setting. **_space_group.name_H-M_alt** and **_space_group.name_H-M_full** give the user the freedom to give the symbol in any setting, but cannot be reliably interpreted by a computer.

Secondly, the SPACE_GROUP category contains information about the symmetry properties of the space group, such as its Laue class, Bravais type and point group.

Thirdly, the SPACE_GROUP category contains information which specifies the setting. Although this is implicit in the Hall symbol or in the list of symmetry operations that are given in the SPACE_GROUP_SYMOP category, it can be made explicit by including the transformation needed to generate the setting used in the CIF from the reference setting specified in the dictionary. The reference setting is defined in two ways: firstly, in the list of allowed values of **_space_group.name_H-M_ref**; and secondly in a concordance correlating the *International Tables* number and the Schoenflies symbol of the space group with the Hermann–Mauguin symbol of the reference setting and the Hall symbol. Either of the latter two can be used to generate the symmetry operations in the reference setting.

Information on several space groups may be looped. In this case, each space group is identified by the item **_space_group.id**, which is a parent to various ***.sg_id** items in the other categories. This allows a number of different space groups, or different settings of the same space group, to be defined within the same CIF.

Although the most elegant way of specifying the symmetry operations of the space group is to use the Hermann–Mauguin symbol of the reference setting or the Hall symbol (depending on the setting), it is common practice to list all the symmetry operations explicitly in a CIF. For each space group these must appear in a loop and so require their own category, SPACE_GROUP_SYMOP. The symmetry operations may be specified in one of two ways, either through a full list of all the operations of the group or through a restricted list of generators which, when multiplied by each other, generate the full list.

The list of symmetry operations may contain the operations of several space groups, the particular space group being identified by **_space_group_symop.sg_id**.

Special positions are looped in the SPACE_GROUP_WYCKOFF category, which permits a description of the properties of each special position of one or more space groups. In the current structure of CIF it is not possible to give all the equivalent positions associated with a particular special position, but these can easily

be generated by applying the symmetry operations of the space group to the representative special position whose coordinates are included. Although the multiplicity and site symmetry of a given special position can be calculated if the symmetry operations are known, the Wyckoff letter cannot be calculated since it is assigned arbitrarily and is setting-independent.

As with the symmetry operations, it is possible to include the special positions of more than one space group, each space group being identified by `_space_group_Wyckoff.sg_id`.

3.8.4. Future developments

Version 1.0 of the symmetry CIF dictionary contains only the basic items needed to define the properties of the three-dimensional space groups. It is only the first step in the definition of a more comprehensive symmetry dictionary. Future versions will define items needed to describe the higher-dimensional symmetries that have recently proved popular for describing modulated structures and quasicrystals, and items to make it easier for computers to explore the relationships between a space group and its super- and subgroups.

The addition of methods in future versions of the DDL will permit the dictionary to include the expressions for calculating each item from other items in the CIF. Methods will be particularly useful in the symmetry CIF dictionary, since almost all its items can be calculated from a single item: a symmetry generator name. The symmetry CIF dictionary is an essential component in the plan to make the suite of CIF dictionaries a self-contained online compendium of crystallographic knowledge.

It is my pleasure to acknowledge the contributions made by members of the working group that prepared the dictionary: Ralf Grosse-Kunstleve, Vojtech Kopsky, Danny Litvin, Gotzon Madariaga, Mois Aroyo, Uri Shmueli, Ad Thiers and Hans Wondratschek.

References

Hall, S. R. & Grosse-Kunstleve, R. W. (2001). *International tables for crystallography*, Vol. B, *Reciprocal space*, edited by U. Shmueli, 2nd ed., Appendix A1.4.2.3. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2002). Vol. A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.