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3.8. Classification and use of symmetry data

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3.8.1. Introduction

Symmetry lies at the heart of crystallography. Volume A of *International Tables for Crystallography* (2002) (*IT* A) is among the most widely consulted crystallographic texts, since it defines the concepts underlying the theory of three-dimensional crystal symmetry and gives detailed descriptions of the 230 different space groups. These descriptions are essential for anyone studying crystals, since no structure report is complete if the space group is not given.

For this reason, the original core CIF dictionary included a small number of the essential items needed to describe the symmetry of a crystal structure. Among these were three different forms of the space-group name (symbol) and a listing of the symmetry operations in algebraic form. This group of items has proved sufficient for the purpose of archiving crystal structures, but it does not readily lend itself to further extension.

Symmetry concepts have precise definitions, which makes them particularly amenable to manipulation by computer. It is therefore natural to consider the ways in which the concepts of space-group theory and practice should be represented in CIF. Possible applications for an extended list of symmetry items in CIF include online access to the tables given in *International Tables for Crystallography* Volume A (properties of space groups), Volume A1 (relationships between space groups) and Volume E (properties of layer and frieze groups), as well as to allow the description of higher-dimensional symmetry in CIFs reporting quasicrystal, magnetic and modulated structures. To be effective, any CIF definitions have to reflect the current state of space-group theory, as well as meeting the needs of future software that will automatically assemble and manipulate information drawn from crystallographic and other databases.

3.8.2. Dictionary design considerations

In 1995, a working group was established to draw up a CIF symmetry dictionary. The group quickly encountered two problems. Firstly, scientists in different fields have different expectations of space-group theory and conflicting requirements for CIF definitions, and secondly the familiar presentation of space groups that works well in a printed book such as *IT* A is not necessarily the best way of presenting the material in a computer-based system. These problems are illustrated by the difficulties that the working group encountered in defining the space-group symbols. Each space group can be fully described only within a particular coordinate system or setting, but most space groups can be represented in many different settings and no one setting is uniquely fitted for this role. Ideally, one would like to have access to representations of the symmetry operations in all possible settings, but this is impractical in a printed book. *IT* A restricts itself to representing the space groups in a small number, often only one, of the many possible settings. However, computers are not limited in the same way, since it is possible to calculate the operations for any desired setting without additional overhead. This is an advantage for experimental crystallographers who like to choose the setting to suit the crystal, but theorists prefer to use the same fixed reference setting for all instances of a space group because it leads to a consistent description of group–subgroup and other relationships between the space groups.

This difficulty is resolved in the CIF symmetry dictionary by recognizing that there are two types of space-group symbol: those such as the Schoenflies symbol and the *International Tables* number that identify the space group without specifying the setting; and those such as the Hall symbol (Hall & Grosse-Kunstleve, 2001) that are symmetry generators and therefore define the space group within a particular setting. The weakness of the setting-independent symbols is that they are labels that carry at best only a limited amount of information about the symmetry. Full details of the symmetry operations can only be found by consulting a concordance that lists the operations in some arbitrarily chosen setting. The weakness of the symmetry generators is that different settings of the same space group require different symbols, making it difficult to recognize when two symbols refer to the same space group. Unfortunately, the widely used Hermann–Mauguin symbols suffer from both weaknesses. They can be used as space-group generators, but they do not cover all possible settings because they contain no information about the choice of origin. This makes them inappropriate for use when all possible settings are needed. But equally they cannot be used as unique space-group identifiers, since many space groups can be described by more than one Hermann–Mauguin symbol. They are not therefore well adapted to computer use, but they are popular because they are easy to interpret and they indicate in a simple way the relationship between the symmetry operations and the axis system.

Because CIF requires a unique and precise definition for any symbol that a program is required to interpret, the working group found it necessary to define different versions of the Hermann–Mauguin symbol. There is a tightly defined version, **`_space_group.name_H-M_ref`**, which can be used to generate the symmetry operations of the reference setting, but only one form of this symbol (that given in the list of values specified by the dictionary) can be used for a given space group. For consistency with earlier work, the reference settings in this list have all been chosen from among those listed in *IT* A. Where there is a choice of settings in *IT* A, the *b*-axis setting is chosen for monoclinic, and the hexagonal setting is chosen for rhombohedral space groups. Where two different origin choices are given, the second (origin at a centre of symmetry) is chosen. A second more loosely defined Hermann–Mauguin symbol, **`_space_group.name_H-M_alt`**, is defined for the benefit of those who like to use the Hermann–Mauguin symbol to indicate the axis system adopted, but as this item does not have a precise definition, it should not be interpreted by a software application. It should be treated as a text string that can be displayed for the benefit of the user.

The symmetry CIF dictionary differs in an important way from the other CIF dictionaries. While the other dictionaries define items that give the results of an experimental measurement, all the items in the symmetry dictionary are either theoretically derivable or, like the reference settings and Wyckoff letters, are arbitrarily

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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

references