1.4. Space groups and their descriptions

B. Souvignier, H. Wondratschek, M. I. Aroyo, G. Chapuis and A. M. Glazer

1.4.1. Symbols of space groups

By H. Wondratschek

1.4.1.1. Introduction

Space groups describe the symmetries of crystal patterns; the point group of the space group is the symmetry of the macroscopic crystal. Both kinds of symmetry are characterized by symbols of which there are different kinds. In this section the space-group numbers as well as the Schoenflies symbols and the Hermann–Mauguin symbols of the space groups and point groups will be dealt with and compared, because these are used throughout this volume. They are rather different in their aims. For the Fedorov symbols, mainly used in Russian crystallographic literature, *cf.* Chapter 3.3. In that chapter the Hermann–Mauguin symbols and their use are also discussed in detail. For computer-adapted symbols of space groups implemented in crystallographic software, such as *Hall symbols* (Hall, 1981*a*,*b*) or *explicit symbols* (Shmueli, 1984), the reader is referred to Chapter 1.4 of *International Tables for Crystallography*, Volume B (2008).

For the definition of space groups and plane groups, *cf.* Chapter 1.3. The plane groups characterize the symmetries of two-dimensional periodic arrangements, realized in sections and projections of crystal structures or by periodic wallpapers or tilings of planes. They are described individually and in detail in Chapter 2.2. Groups of one- and two-dimensional periodic arrangements embedded in two-dimensional and three-dimensional space are called *subperiodic groups*. They are listed in Vol. E of *International Tables for Crystallography* (2010) (referred to as *IT* E) with symbols similar to the Hermann–Mauguin symbols of plane groups and space groups, and are related to these groups as their subgroups. The space groups *sensu stricto* are the symmetries of periodic arrangements in three-dimensional space, *e.g.* of normal crystals, see also Chapter 1.3. They are described individually and in detail in the space-group tables of Chapter 2.3. In the following, if not specified separately, both space groups and plane groups are covered by the term *space group*.

The description of each space group in the tables of Chapter 2.3 starts with two headlines in which the different symbols of the space group are listed. All these names are explained in this section with the exception of the data for *Patterson symmetry* (*cf.* Chapter 1.6 and Section 2.1.3.5 for explanations of Patterson symmetry).

1.4.1.2. Space-group numbers

The space-group numbers were introduced in *International Tables for X-ray Crystallography* (1952) [referred to as *IT* (1952)] for plane groups (Nos. 1–17) and space groups (Nos. 1–230). They provide a short way of specifying the type of a space group uniquely, albeit without reference to its symmetries. They are particularly convenient for use with computers and have been in use since their introduction.

There are no numbers for the point groups.

1.4.1.3. Schoenflies symbols

The Schoenflies symbols were introduced by Schoenflies (1891, 1923). They describe the point-group type, also known as the geometric crystal class or (for short) crystal class (*cf.* Section 1.3.4.2), of the space group geometrically. The different space-group types within the same crystal class are denoted by a superscript index appended to the point-group symbol.

1.4.1.3.1. Schoenflies symbols of the crystal classes

Schoenflies derived the point groups as groups of crystallographic symmetry operations, but described these crystallographic point groups geometrically by their representation through axes of rotation or rotoreflection and reflection planes (also called mirror planes), *i.e.* by *geometric elements*; for geometric elements of symmetry elements, *cf.* Section 1.2.3, de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000). Rotation axes dominate the description and planes of reflection are added when necessary. Rotoreflection axes are also indicated when necessary. The orientation of a reflection plane, whether *horizontal*, *vertical* or *diagonal*, refers to the plane itself, not to its normal.

A coordinate basis may be chosen by the user: the basis vectors start at the origin which is placed in front of the user. The basis vector **c** points vertically upwards, the basis vectors **a** and **b** lie

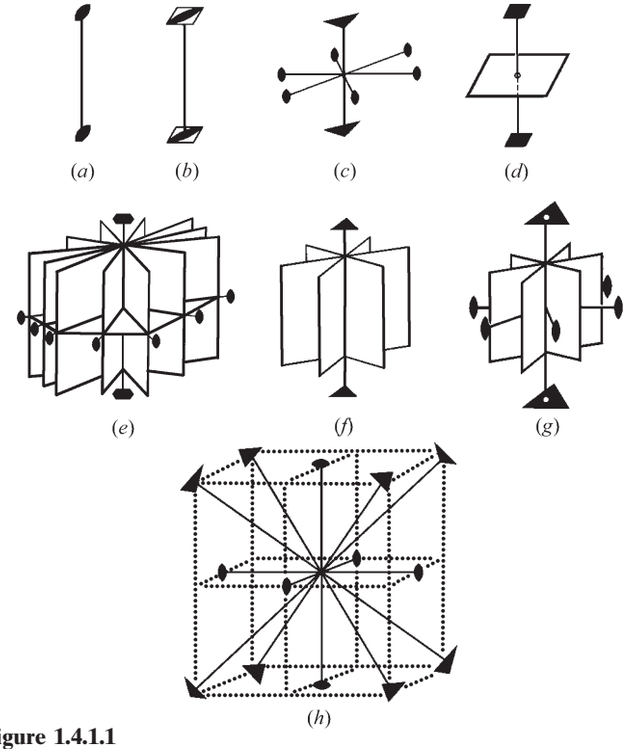

Figure 1.4.1.1
Symmetry-element diagrams of some point groups [adapted from Vainshtein (1994)]. The point groups are specified by their Schoenflies and Hermann–Mauguin symbols. (*a*) $C_2 = 2$, (*b*) $S_4 = \bar{4}$, (*c*) $D_3 = 32$, (*d*) $C_{4h} = 4/m$, (*e*) $D_{6h} = 6/m\,2/m\,2/m$, (*f*) $C_{3v} = 3m$, (*g*) $D_{3d} = \bar{3}\,2/m$, (*h*) $T = 23$. [The cubic frame in part (*h*) has no crystallographic meaning: it has been included to aid visualization of the orientation of the symmetry elements.]

more or less horizontal; the basis vector **a** pointing at the user, **b** pointing to the user's right-hand side, *i.e.* the basis vectors **a**, **b** and **c** form a *right-handed* set. Such a basis will be called a *conventional crystallographic basis* in this chapter. (In the usual basis of mathematics and physics the basis vector **a** points to the right-hand side and **b** points away from the user.) The lengths of the basis vectors, the inclination of the **ab** plane relative to the **c** axis and the angles between the basis vectors are determined by the symmetry of the point group and the specific values of the lattice parameters of the crystal structure.

The letter C is used for *cyclic groups* of rotations around a rotation axis which is conventionally **c**. The order n of the rotation is appended as a subscript index: C_n; Fig. 1.4.1.1(a) represents C_2. The values of n that are possible in the rotation symmetry of a crystal are 1, 2, 3, 4 and 6 (*cf.* Section 1.3.3.1 for a discussion of this basic result). The axis of an n-fold rotoreflection, *i.e.* an n-fold rotation followed or preceded by a reflection through a plane perpendicular to the rotation axis (such that neither the rotation nor the reflection is in general a symmetry operation) is designated by S_n, see Fig. 1.4.1.1(b) for S_4.

The following types of point groups exist:

(1) cyclic groups

(a) of rotations (C):

$$C_1,\ C_2,\ C_3,\ C_4,\ C_6;$$

(b) of rotoreflections (S, for the names in parentheses see later):

$$S_1\ (=C_{1h}=C_s),\ S_2\ (=C_i),\ S_3\ (=C_{3h}),\ S_4,\ S_6\ (=C_{3i}).$$

(2) In dihedral groups D_n an n-fold (vertical) rotation axis is accompanied by n symmetry-equivalent horizontal twofold rotation axes. The symbols are D_2 [in older literature, as in *IT* (1952), one also finds V instead of D_2, taken from the *Vierergruppe* of Klein (1884)], $D_3,\ D_4,\ D_6$; D_3 is visualized in Fig. 1.4.1.1(c).

(3) Other crystallographic point groups can be constructed by a C_n rotation axis or a D_n combination of rotation axes with a horizontal symmetry plane, leading to symbols C_{nh} or D_{nh}:

$$C_{2h}, C_{3h}, C_{4h}, C_{6h}, D_{2h}, D_{3h}, D_{4h}, D_{6h}.$$

The point groups C_{4h} and D_{6h} are represented by Figs. 1.4.1.1(d) and 1.4.1.1(e).

(4) Vertical rotation axes C_n can be combined with a vertical reflection plane, leading to n symmetry-equivalent vertical reflection planes (denoted v) which all contain the rotation axis:

$$C_{2v},\ C_{3v},\ C_{4v},\ C_{6v}$$

with Fig. 1.4.1.1(f) for C_{3v}.

(5) Combinations D_n of rotation axes may be combined with vertical reflection planes which bisect the angles between the horizontal twofold axes, such that the vertical planes (designated by the index d for 'diagonal') alternate with the horizontal twofold axes:

$$D_{2d} \text{ with } n=2 \text{ or } D_{3d} \text{ with } n=3;$$

see Fig. 1.4.1.1(g) for D_{3d}. In both point groups rotoreflections S_{2n}, *i.e.* S_4 or S_6, occur. Note that the classification of crystal classes into crystal systems follows the order of rotoinversions $\overline{N}$, not that of rotoreflections S_n (*cf.* Section 1.2.1 for the definition of rotoinversions). Therefore, D_{2d} is tetragonal ($S_4 \sim \overline{4}$) and D_{3d} is trigonal because of $S_6^5 = \overline{3}$). Analogously, C_{3h} and D_{3h} are hexagonal because they contain $S_3 \sim \overline{6}$. The point groups D_{4d} and D_{6d} are not crystallographic as they contain noncrystallographic eightfold or 12-fold rotoreflections S_8 or S_{12}.

(6) In all these groups the directions of the vectors $\pm$**c** are not equivalent to any other directions. There are, however, also cubic point groups and thus cubic space groups in which the basis vector **c** is symmetry-equivalent to both basis vectors **a** and **b**. T, T_h and T_d can be derived from the rotation group T of the tetrahedron, see Fig. 1.4.1.1(h). O and O_h can be derived from the rotation group O of the octahedron. The indices h and d have the same meaning as before.

(7) Some of these symbols are no longer used but are replaced by more visual ones. S_1 describes a reflection through a horizontal plane, it is replaced now by C_{1h} or by C_s; S_2 describes an inversion in a centre, it is replaced by C_i. The symbol S_3 describes the same arrangement as C_{3h} and is thus not used. S_6 contains an inversion centre combined with a threefold rotation axis and is replaced by C_{3i}.

The description of crystal classes using Schoenflies symbols is intuitive and much more graphic than that by Hermann–Mauguin symbols. It is useful for morphological studies investigating the symmetry of the ideal shape of crystals. Schoenflies symbols of crystal classes are also still used traditionally by physicists and chemists, in particular in spectroscopy and quantum chemistry.

1.4.1.3.2. Schoenflies symbols of the space groups

Different space groups of the same crystal class are distinguished by their superscript index, for example C_1^1; $D_{2h}^1, D_{2h}^2, \ldots, D_{2h}^{28}$ or $O_h^1, \ldots, O_h^{10}$.

Schoenflies symbols display the space-group symmetry only partly. Therefore, they are nowadays rarely used for the description of the symmetry of crystal structures. In comparison with the Schoenflies symbols, the Hermann–Mauguin symbols are more indicative of the space-group symmetry and that of the crystal structures.

1.4.1.4. Hermann–Mauguin symbols of the space groups

1.4.1.4.1. Introduction

The Hermann–Mauguin symbols, abbreviated as HM symbols in the following sections, were proposed by Hermann (1928, 1931) and Mauguin (1931), and introduced to the *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) according to the decision of the corresponding Programme Committee (Ewald, 1930). There are different kinds of HM symbols of a space group. One distinguishes *short HM symbols*, *full HM symbols* and *extended HM symbols*. The *full HM symbols* will be the basis of this description. They form the most transparent kind of HM symbols and their use will minimize confusion, especially for those who are new to crystallography.

As the name suggests, the *short HM symbols* are mostly shortened versions of the full HM symbols: some symmetry information of the full HM symbols is omitted such that these symbols are more convenient in daily use. The full HM symbol can be reconstructed from the short symbol. In the *extended HM symbols* the symmetry of the space group is listed in a more complete fashion (*cf.* Section 1.5.4). They are rarely used in crystallographic practice.

In the next section general features of the HM symbols will be discussed. Thereafter, the HM symbols for each crystal system will be presented in a separate section, because the appearance of