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

the HM symbols depends strongly on the crystal system to which the space group belongs.

1.4.1.4.2. General aspects

The Hermann–Mauguin symbol for a space group consists of a sequence of letters and numbers, here called the *constituents of the HM symbol*. The first constituent is always a symbol for the conventional cell of the translation lattice of the space group (*cf.* Section 1.3.2.1 for the definition of the translation lattice); the following constituents, namely rotations, screw rotations, rotoinversions, reflections and glide reflections, are marked by conventional symbols, *cf.* Table 2.1.2.1.[1] Together with the generating translations of the lattice, the set of these symmetry operations forms a *set of generating symmetry operations* of the space group. The space group can thus be generated from its HM symbol.

The symmetry operations of the constituents are referred to the lattice basis that is used conventionally for the crystal system of the space group. The kind of symmetry operation can be read from its symbol; the orientation of its geometric element, *cf.* de Wolff *et al.* (1989, 1992), *i.e.* its invariant axis or plane normal, can be concluded from the position of the corresponding constituent in the HM symbol, as the examples in the following sections will show. The origin is not specified. It is chosen by the user, who selects it in such a way that the matrices of the symmetry operations appear in the most convenient form. This is often, but not necessarily, the conventional origin chosen in the space-group tables of this volume. The choice of a different origin may make other tasks, *e.g.* the derivation of the space group from its generators, particularly easy and transparent.

The first constituent (the lattice symbol) characterizes the lattice of the space group referred to the conventional coordinate system. (Each lattice can be referred to a lattice basis, also called a *primitive basis*: the lattice vectors have only integer coefficients and the lattice is called a *primitive lattice*.) Lattice vectors with non-integer coefficients can occur if the lattice is referred to a non-primitive basis. In this way similarities and relations between different space-group types are emphasized.

The lattice symbol of a primitive basis consists of an upper-case letter *P* (**p**rimitive). Lattices with conventional non-primitive bases are called *centred lattices*, *cf.* Section 1.3.2.4 and Table 2.1.1.2. For these other letters are used: if the **ab** plane of the unit cell is centred with a lattice vector $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, the letter is *C*; for **ca** centring [$(\frac{1}{2}(\mathbf{c}+\mathbf{a})$ as additional *centring vector*] the letter is *B*, and *A* is the letter for centring the **bc** plane of the unit cell by $\frac{1}{2}(\mathbf{b}+\mathbf{c})$. The letter is *F* for centring all side faces of the cell with centring vectors $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(\mathbf{c}+\mathbf{a})$ and $\frac{1}{2}(\mathbf{b}+\mathbf{c})$. It is *I* (German: ***i**nnenzentriert*) for body centring by the vector $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ and *R* for the rhombohedral centring of the hexagonal cell by the vectors $\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$ and $\frac{1}{3}(\mathbf{a}+2\mathbf{b}+2\mathbf{c})$. In 1985, the letter *S* was introduced as a setting-independent 'centring symbol' for monoclinic and orthorhombic Bravais lattices (*cf.* de Woff *et al.*, 1985).

To describe the structure of the HM symbols the introduction of the term *symmetry direction* is useful.

Definition

A direction is called a *symmetry direction* of a crystal structure if it is parallel to an axis of rotation, screw rotation or rotoinversion or if it is parallel to the normal of a reflection or glide-reflection plane. A symmetry direction is thus the direction of the geometric element of a symmetry operation when the normal of a symmetry plane is used for the description of its orientation.

The corresponding symmetry operations [the *element set* of de Wolff *et al.* (1989 & 1992)] specify the type of the symmetry direction. The symmetry direction is always a lattice direction of the space group; the shortest lattice vector in the symmetry direction will be called **q**.

If **q** represents both a rotation or screw rotation and a reflection or glide reflection, then their symbols are connected in the HM symbol by a slash '/', *e.g.* 2/*m* or $4_1/a$ *etc*.

The symmetry directions of a space group form *sets of equivalent symmetry directions* under the symmetry of the space group. For example, in a cubic space group the **a**, **b** and **c** axes are equivalent and form the set of six directions ⟨100⟩: [100], [$\bar{1}$00], [010] *etc.* Another set of equivalent directions is formed by the eight space diagonals ⟨111⟩: [111], [1$\bar{1}\bar{1}$], ... If there are twofold rotations around the twelve face diagonals ⟨110⟩, as in the space group of the crystal structure of NaCl, ⟨110⟩ forms a third set of 12 symmetry directions.[2]

Instead of listing the symmetry operations (element set) for each symmetry direction of a set of symmetry directions, it is sufficient to choose one *representative direction of the set*. In the HM symbol, generators for the element set of each representative direction are listed.

It can be shown that there are zero (triclinic space groups), one (monoclinic), up to two (trigonal and rhombohedral) or up to three (most other space groups) sets of symmetry directions in each space group and thus zero, one, two or three representative symmetry directions.

The non-translation generators of a symmetry direction may include only one kind of symmetry operation, *e.g.* for twofold rotations 2 in space group *P*121, but they may also include several symmetry operations, *e.g.* 2, 2_1, *m* and *a* in space group *C*12/*m*1. To search for such directions it is helpful simply to look at the space-group diagrams to find out whether more than one kind of symmetry operation belongs to the generators of a symmetry direction. In general, only the simplest symbols are listed (*simplest-operation rule*): if we use '>' to mean '*has priority*', then pure rotations > screw rotations; pure rotations > rotoinversions; reflection $m > a, b, c > n$.[3] The space group mentioned above is conventionally called *C*12/*m*1 and not $C12_1/m1$ or $C12/a1$ or $C12_1/a1$.

The position of a plane is fixed by one parameter if its orientation is known. On the other hand, fixing an axis of known direction needs two parameters. Glide components also show two-dimensional variability, whereas there is only one parameter

[1] According to the recommendations of the International Union of Crystallography Ad Hoc Committee on the Nomenclature of Symmetry (de Wolff *et al.*, 1992), the characters appearing after the lattice letter in the HM symbol of a space group should represent symmetry elements, which is reflected, for example, in the introduction of the '*e*-glide' notation in the HM space-group symbols. To avoid misunderstandings, it is worth noting that in the following discussion of the HM symbolism, the author preferred to keep strictly to the original idea according to which the characters of the HM symbols were meant to represent (generating) symmetry operations of the space group, and not symmetry elements.

[2] The numbers listed are those for bipolar directions, for which direction and opposite direction are equivalent. For the corresponding polar directions in cubic space groups only the four equivalent polar directions ⟨111⟩ or ⟨1$\bar{1}\bar{1}$⟩ of the tetrahedron occur.

[3] The 'symmetry-element' interpretation of the constituents of the HM symbols (*cf.* footnote 1[1]) results in the following modification of the 'simplest-operation' rule [known as the 'priority rule', *cf.* Section 4.1.2.3 of *International Tables for Crystallography*, Volume A (2002) (referred to as *IT* A5)]: When more than one kind of symmetry element exists in a given direction, the choice of the corresponding symbols in the space-group symbol is made in order of descending priority $m > e > a, b, c > n$, and rotation axes before screw axes.