International Tables for Crystallography (2016). Vol. A, Section 1.4.1, pp. 42–50.

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

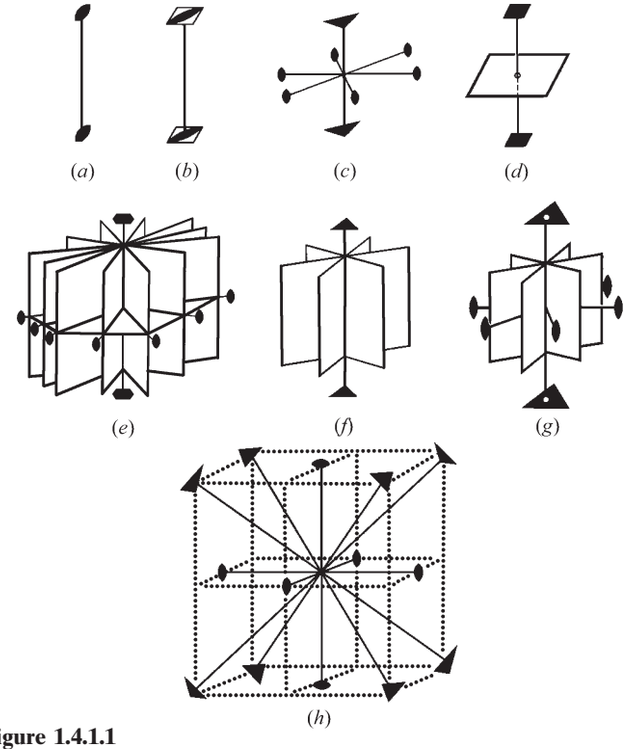

Figure 1.4.1.1
Symmetry-element diagrams of some point groups [adapted from Vainshtein (1994)]. The point groups are specified by their Schoenflies and Hermann–Mauguin symbols. (*a*) $C_2 = 2$, (*b*) $S_4 = \bar{4}$, (*c*) $D_3 = 32$, (*d*) $C_{4h} = 4/m$, (*e*) $D_{6h} = 6/m\,2/m\,2/m$, (*f*) $C_{3v} = 3m$, (*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

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.

of a screw component. Therefore, reflections and glide reflections can better express the geometric relations between the symmetry operations than can rotations and screw rotations; reflections and glide reflections are more important for HM symbols than are rotations and screw rotations. The latter are frequently omitted to form short HM symbols from the full ones.

The second part of the *full HM symbol* of a space group consists of one position for each of up to three representative symmetry directions. To each position belong the generating symmetry operations of their representative symmetry direction. The position is thus occupied either by a rotation, screw rotation or rotoinversion and/or by a reflection or glide reflection.

The representative symmetry directions are different in the different crystal systems. For example, the directions of the basis vectors **a**, **b** and **c** are symmetry independent in orthorhombic crystals and are thus all representative, whereas **a** and **b** are symmetry equivalent and thus dependent in tetragonal crystals. All three directions are symmetry equivalent in cubic crystals; they belong to the same set and are represented by one of the directions. Therefore, the symmetry directions and their sequence in the HM symbols depend on the crystal system to which the crystal and thus its space group belongs.

Table 1.4.1.1
The structure of the Hermann–Mauguin symbols for the space groups

The positions of the representative symmetry directions for the different crystal systems are given. The description of the non-translational part of the HM symbol is always preceded by the lattice symbol, which in conventional settings is *P*, *A*, *B*, *C*, *F*, *I* or *R*. For monoclinic **b** setting and monoclinic **c** setting, *cf.* Section 1.4.1.4.4; the primitive hexagonal lattice is called *H* in this table.

Crystal system	First position	Second position	Third position
Triclinic (anorthic)	1 or $\bar{1}$	—	—
Monoclinic **b** setting Monoclinic **c** setting	1 1	**b** 1	1 **c**
Orthorhombic	**a**	**b**	**c**
Tetragonal	**c**	**a**	$\mathbf{a}-\mathbf{b}$
Trigonal *H* lattice	**c** **c**	**a** or 1	1 $\mathbf{a}-\mathbf{b}$
Trigonal, *R* lattice, hexagonal coordinates Trigonal, *R* lattice, rhombohedral coordinates	$\mathbf{c}_H$ $\mathbf{a}_R+\mathbf{b}_R+\mathbf{c}_R$	$\mathbf{a}_H$ or $\mathbf{a}_R-\mathbf{b}_R$	— —
Hexagonal	**c**	**a**	$\mathbf{a}-\mathbf{b}$
Cubic	**c**	$\mathbf{a}+\mathbf{b}+\mathbf{c}$	$\mathbf{a}-\mathbf{b}$

Table 1.4.1.1 gives the positions of the representative lattice-symmetry directions in the HM symbols for the different crystal systems.

Examples of full HM symbols are (from triclinic to cubic) $P\bar{1}$, $P12/c1$, $A112/m$, $F2/d2/d2/d$, $I4_1/a$, $P4/m2_1/n2/c$, $P\bar{3}$, $P3m1$, $P3_112$, $R\bar{3}2/c$, $P6_3/m$, $P6_122$ and $F4_132$.

There are crystal systems, for example tetragonal, for which the high-symmetry space groups display symmetry in all symmetry directions whereas lower-symmetry space groups display symmetry in only some of them. In such cases, the symmetry of the 'empty' symmetry direction is denoted by the constituent 1 or it is simply omitted. For example, instead of three symmetry directions in $P4mm$, there is only one in $I4_1/a11$, for which the HM symbol is usually written $I4_1/a$. However, in some trigonal space groups the designation of a symmetry direction by '1' ($P3_112$) is necessary to maintain the uniqueness of the HM symbols.[4]

The HM symbols can not only describe the space groups in their conventional settings but they can also indicate the setting of the space group relative to the conventional coordinate system mentioned in Section 1.4.1.3.1. For example, the orthorhombic space group $P2/m2/n2_1/a$ may appear as $P2/n2/m2_1/b$ or $P2/n2_1/c2/m$ or $P2_1/c2/n2/m$ or $P2_1/b2/m2/n$ or $P2/m2_1/a2/n$ depending on its orientation relative to the conventional coordinate basis. On the one hand this is an advantage, because the HM symbols include some indication of the orientation of the space group and form a more powerful tool than being just a space-group nomenclature. On the other hand, it is sometimes not easy to recognize the space-group type that is described by an unconventional HM symbol. In Section 1.4.1.4.5 an example is provided which deals with this problem.

[4] In the original HM symbols the constituent '1' was avoided by the use of different centred cells.

The full HM symbols describe the symmetry of a space group in a transparent way, but they are redundant. They can be shortened to the *short HM symbols* such that the set of generators is reduced to a necessary set. Examples will be displayed for the different crystal systems. The *conventional short HM symbols* still provide a unique description and enable the generation of the space group. For the monoclinic space groups with their many conventional settings they are not variable and are taken as standard for their space-group types. Monoclinic short HM symbols may look quite different from the full HM symbol, *e.g.* Cc instead of $A1n1$ or $I1a1$ or $B11n$ or $I11b$.

The *extended HM symbols* display the additional symmetry that is often generated by lattice centrings. The full HM symbol denotes only the simplest symmetry operations for each symmetry direction, by the 'simplest symmetry operation' rule; the other operations can be found in the extended symbols, which are treated in detail in Section 1.5.4 and are listed in Tables 1.5.4.3 (plane groups) and 1.5.4.4 (space groups).

From the HM symbol of the space group, the full or short *HM symbol for a crystal class* of a space group is obtained easily: one omits the lattice symbol, cancels all screw components such that only the symbol for the rotation is left and replaces any letter for a glide reflection by the letter *m* for a reflection. Examples are $P2_1/b2_1/a2/m \rightarrow 2/m2/m2/m$ and $I4_1/a11 \rightarrow 4/m$.

If one is not yet familiar with the HM symbols, it is recommended to start with the orthorhombic space groups in Section 1.4.1.4.5. In the orthorhombic crystal system all crystal classes have the same number of symmetry directions and the HM symbols are particularly transparent. Therefore, the orthorhombic HM symbols are explained in more detail than those of the other crystal systems.

The following discussion treats mainly the HM symbols of space groups in conventional settings; for non-conventional descriptions of space groups the reader is referred to Chapter 1.5.

1.4.1.4.3. Triclinic space groups

There is no symmetry direction in a triclinic space group. Therefore, the basis vectors of a triclinic space group can always be chosen to span a primitive cell and the HM symbols are $P1$ (without inversions) and $P\bar{1}$ (with inversions). The HM symbol

$P\bar{1}$ is the only one which displays the inversion $\bar{1}$ explicitly. Sometimes non-conventional centred lattice descriptions may be used, especially when comparing crystal structures.

1.4.1.4.4. Monoclinic space groups

Monoclinic space groups have exactly one symmetry direction, often called *the monoclinic axis*. The *b* axis is the symmetry direction of the (most frequently used) conventional setting, called the *b*-axis setting. Another conventional setting has **c** as its symmetry direction (*c*-axis setting). In earlier literature, the unique-axis *c* setting was called the first setting and the unique-axis *b* setting the second setting (*cf.* Section 2.1.3.15). In addition to the primitive lattice *P* there is a centred lattice which is taken as *C* in the *b*-axis setting, *A* in the *c*-axis setting. The (possible) glide reflections are *c* (or *a*). In this volume, more settings are described, *cf.* Sections 1.5.4 and 2.1.3.15 and the space-group tables of Chapter 2.3.

The full HM symbol consists of the lattice symbol and three possible positions for the symmetry directions. The symmetry in the **a** direction is described first, followed by the symmetry in the **b** direction and last in the **c** direction. The two positions of the HM symbol that are not occupied by the monoclinic symmetry direction are marked by 1. The symbol is thus similar to the orthorhombic HM symbol and the monoclinic axis is clearly visible. *P*1*m*1 or *P*11*m* may designate the same space group but in different settings. *Pm*11 is a possible but not conventional setting.

The short HM symbols of the monoclinic space groups are independent of the setting of the space group. They form the *monoclinic standard symbols* and are not variable: *P*2, $P2_1$, *C*2, *Pm*, *Pc*, *Cm*, *Cc*, *P*2/*m*, $P2_1/m$, *C*2/*m*, *P*2/*c*, $P2_1/c$ and *C*2/*c*. Altogether there are 13 monoclinic space-group types.

There are several reasons for the many conventional settings.

(1) As only one of the three coordinate axes is fixed by symmetry, there are two conventions related to the possible permutations of the other axes.
(2) The sequence of the three coordinate axes may be chosen because of the lengths of the basis vectors, *i.e.* not because of symmetry.
(3) If two different crystal structures have related symmetries, one being a subgroup of the other, then it is often convenient to choose a non-conventional setting for one of the structures to make their structural relations transparent. Such similarity happens in particular in substances that are related by a non-destructive phase transition. Monoclinic space groups are particularly flexible in their settings.

1.4.1.4.5. Orthorhombic space groups

To the orthorhombic crystal system belong the crystal classes 222, *mm*2 and 2/*m* 2/*m* 2/*m* with the Bravais types of lattices *P*, *C*, *A*, *F* and *I*. Four space groups with a *P* lattice belong to the crystal class 222, ten to *mm*2 and 16 to 2/*m* 2/*m* 2/*m*. Each of the basis vectors marks a symmetry direction; the lattice symbol is followed by characters representing the symmetry operations with respect to the symmetry directions along **a**, **b** and **c**.

We start with the full HM symbols. For a space group of crystal class 222 with a *P* lattice the HM symbol is thus '$PR_1R_2R_3$', where R_1, R_2, $R_3 = 2$ or 2_1. Conventionally one chooses a setting with the symbols *P*222, $P222_1$, $P2_12_12$ and $P2_12_12_1$.

For the generation of the space groups of this crystal class only two non-translational generators are necessary, say R_1 and R_2. However, it is not possible to indicate in the HM symbol whether the axes R_1 and R_2 intersect or not. This is decided by the third (screw) rotation R_3: if $R_3 = R_1R_2 = 2$, the axes R_1 and R_2 intersect, if $R_3 = 2_1$, they do not. For this reason, R_3 is sometimes called an *indicator*. However, any two of the three rotations or screw rotations can be taken as the generators and the third one is then the indicator. Mathematically each element of a generating set is a generator independent of its possible redundancy.

In the space groups of crystal class *mm*2 the two reflections or glide reflections are the generators, the twofold rotation or screw rotation is generated by composition of the (glide) reflections. The position of the rotation axis relative to the intersection line of the two planes as well as its screw component are determined uniquely by the glide components of the reflections or glide reflections.

The rotation or screw rotation in the HM symbols of space groups of the crystal class *mm*2 could be omitted, and were omitted in older HM symbols. Nowadays they are included to make the orthorhombic HM symbols more homogeneous. Conventional symbols are, among others, *Pmm*2, $Pmc2_1$, *Pba*2 and $Pca2_1$.

The 16 space groups with a *P* lattice in crystal class 2/*m* 2/*m* 2/*m* are similarly obtained by starting with the letter *P* and continuing with the point-group symbol, modified by the possible replacements 2_1 for 2 and *a*, *b*, *c* or *n* for *m*. The conventional symbols are, among others, *P*2/*m* 2/*m* 2/*m*, $P2_1/m\,2/m\,2/a$, $P2/m\,2/n\,2_1/a$, $P2_1/b\,2_1/a\,2/m$ or $P2_1/n\,2_1/m\,2_1/a$. The symbols $P2/m\,2/n\,2_1/a$ and $P2_1/n\,2_1/m\,2_1/a$ designate different space-group types, as is easily seen by looking at the screw rotations: $P2/m\,2/n\,2_1/a$ has screw axes in the direction of **c** only, $P2_1/n\,2_1/m\,2_1/a$ has screw axes in all three symmetry directions.

If the lattice is centred, the constituents in the same symmetry direction are not unique. In this case, according to the 'simplest symmetry operation' rule, in general the simplest operation is chosen, *cf.* Section 1.5.4.

Examples

In the HM symbol $C2/m\,2/c\,2_1/m$ there are in addition 2_1 screw rotations in the first two symmetry directions; additional glide reflections *b* occur in the first, and *n* in the second and third symmetry directions.

In $I2/b\,2/a\,2/m$, all rotations 2 are accompanied by screw rotations 2_1; *b* and *a* are accompanied by *c* and *m* is accompanied by *n*. The symmetry operations that are not listed in the full HM symbol can be derived by composition of the listed operations with a centring translation, *cf.* Section 1.4.2.4.

There are two exceptions to the 'simplest symmetry operation' rule. If the *I* centring is added to the *P* space groups of the crystal class 222, one obtains two different space groups with an *I* lattice, each has 2 and 2_1 operations in each of the symmetry directions. One space group is derived by adding the *I* centring to the space group *P*222, the other is obtained by adding the *I* centring to a space group $P2_12_12_1$. In the first case the twofold axes intersect, in the second they do not. According to the rules both should get the HM symbol *I*222, but only the space group generated from *P*222 is named *I*222, whereas the space group generated from $P2_12_12_1$ is called $I2_12_12_1$. The second exception occurs among the cubic space groups and is due to similar reasons, *cf.* Section 1.4.1.4.8.

The *short HM symbols* for the space groups of the crystal classes 222 and *mm*2 are the same as the full HM symbols. In the short HM symbols for the space groups of the crystal class 2/*m* 2/*m* 2/*m* the symbols for the (screw) rotations are omitted, resulting in the short symbols *Pmmm*, *Pmma*, *Pmna*, *Pbam*, *Pnma*, *Cmcm* and *Ibam* for the space groups mentioned above.

These are HM symbols of space groups in conventional settings. It is less easy to find the conventional HM symbol and the space-group type from an unconventional short HM symbol. This may be seen from the following example:

Question: Given the short HM symbols *Pman*, *Pmbn* and *Pmcn*, what are the conventional descriptions of their space-group types, and are they identical or different?

Answer: A glance at the HM symbols shows that the second symbol does not describe any space-group type at all. The second symmetry direction is **b**; the glide plane is perpendicular to it and the glide component may be $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{c}$ or $\frac{1}{2}(\mathbf{c}+\mathbf{a})$, but not $\frac{1}{2}\mathbf{b}$.

In this case it is convenient to define the intersection of the three (glide) reflection planes as the site of the origin. Then all translation components of the generators are zero except the glide components.

(1) *Pman*. If one names the three (glide) reflections according to the directions of their normals by m_{100}, a_{010} and n_{001}, then $a_{010}n_{001} = 2_{100}$, $m_{100}a_{010} = 2_{001}$, while the composition $n_{001}m_{100}$ results in a 2_1 screw rotation along [010].

Clearly, the unconventional full HM symbol is $P\,2/m\,2_1/a\,2/n$. The procedure for obtaining from this symbol the conventional HM symbol $P\,2/m\,2/n\,2_1/a$ (or short symbol *Pmna*) with the origin at the inversion centre is described in Chapter 1.5.

(2) *Pmcn*. Using a nomenclature similar to that of (1), one obtains 2_1 screw axes along [100], [010] and [001] by the compositons $c_{010}n_{001}$, $n_{001}m_{100}$ and $m_{100}c_{010}$, respectively. Thus the unconventional full HM symbol is $P\,2_1/m\,2_1/c\,2_1/n$. Again, the procedure of Chapter 1.5 results in the full HM symbol $P\,2_1/n\,2_1/m\,2_1/a$ or the short symbol *Pnma*. The full HM symbols show that the two space-group types are different.

1.4.1.4.6. Tetragonal space groups

There are seven tetragonal crystal classes. The lattice may be *P* or *I*. The space groups of the three crystal classes 4, $\overline{4}$ and 4/*m* have only one symmetry direction, [001]. The other four classes, 422, 4*mm*, $\overline{4}2m$ and $4/m\,2/m\,2/m$ display three symmetry directions which are listed in the sequence [001], [100] and $[1\bar{1}0]$.[5]

1.4.1.4.6.1. Tetragonal space groups with one symmetry direction

In the space groups of the crystal class 4, rotation or screw rotation axes run in direction [001]; in the space groups of crystal class $\overline{4}$ these are rotoinversion axes $\overline{4}$; and in crystal class 4/*m* both occur. The rotation 4 of the point group may be replaced by screw rotations 4_1, 4_2 or 4_3 in the space groups with a *P* lattice. If the lattice is *I*-centred, 4 and 4_2 or 4_1 and 4_3 occur simultaneously, together with $\overline{4}$ rotoinversions.

In the space groups of crystal class 4/*m* with a *P* lattice, the rotations 4 can be replaced by the screw rotations 4_2 and the reflection *m* by the glide reflection *n* such that four space-group types with a *P* lattice exist: *P*4/*m*, $P4_2/m$, *P*4/*n* and $P4_2/n$. Two more are based on an *I* lattice: *I*4/*m* and $I4_1/a$. In all these six space groups the short HM symbols and full HM symbols are the same.

[5] One usually chooses $[1\bar{1}0]$ as the representative direction and not the equivalent direction [110], in analogy to the cases of trigonal and hexagonal space groups where $[1\bar{1}0]$ is the representative of the set of tertiary symmetry directions, while $[\bar{1}10]$ (or [110]) belongs to the set of secondary symmetry directions, *cf.* Table 2.1.3.1.

1.4.1.4.6.2. Tetragonal space groups with three symmetry directions

There are four crystal classes with three symmetry directions each. In the corresponding space-group symbols the constituents 2, 4 and *m* may be replaced by 2_1, 4_k with $k = 1$, 2 or 3, and *a*, *b*, *c*, *n* or *d*, respectively. The constituent $\overline{4}$ persists. Full HM symbols of space groups are, among others, $P4_22_12$, $P4_2bc$, $P\overline{4}2c$ and $I\,4_1/a\,2/c\,2/d$.

The full and short HM symbols agree for the space groups that belong to the crystal classes 422, 4*mm* and $\overline{4}2m$. Only for the space groups of $4/m\,2/m\,2/m$ have the short HM symbols lost their twofold rotations or screw rotations leading, *e.g.*, to the symbol $I4_1/acd$ instead of $I\,4_1/a\,2/c\,2/d$.

Example

In *P*4*mm*, to the primary symmetry direction [001] belong the rotation 4 and its powers, to the secondary symmetry direction [100] belongs the reflection m_{100}. However, in the tertiary symmetry direction $[1\bar{1}0]$, there occur reflections *m* and glide reflections *g* with a glide vector $\frac{1}{2}(\mathbf{a}+\mathbf{b})$. Such glide reflections are not listed in the 'symmetry operations' blocks of the space-group tables if they are composed of a representing *general position* and an integer translation, as happens here (*cf.* Section 1.4.2.4 and Section 1.5.4 for a detailed discussion of the additional symmetry operations generated by combinations with integer translations). Glide reflections may have complicated glide vectors. If these do not fit the labels *a*, *b*, *c*, *n* or *d*, they are frequently called *g*.

1.4.1.4.7. Trigonal, hexagonal and rhombohedral space groups

Hexagonal and trigonal space groups are referred to a hexagonal coordinate system *P* with basis vector $\mathbf{c} \perp (\mathbf{a}, \mathbf{b})$. The basis vectors **a** and **b** span a hexagonal net and form an angle of 120°. The sequence of the representatives of the (up to three) symmetry directions is [001], [100] and $[1\bar{1}0]$. Usually, the seven trigonal space groups of the rhombohedral lattice system (or *rhombohedral space groups* for short) are described either with respect to a hexagonal coordinate system (triple hexagonal cell) or to a rhombohedral coordinate system (primitive rhombohedral cell).

1.4.1.4.7.1. Trigonal space groups

Trigonal space groups are characterized by threefold rotation or screw rotation or rotoinversion axes in [001]. There may be in addition 2 and 2_1 axes in [100] or $[1\bar{1}0]$, but only in one of these two directions. The same holds for reflections *m* or glide reflections *c*. The different possibilities are:

(1) There are only threefold axes 3 or 3_1 or 3_2 or $\overline{3}$. The short and the full HM symbols are *P*3, $P3_1$, $P3_2$, $P\overline{3}$.

(2) There are in addition horizontal twofold axes. Their direction is either [100] or $[1\bar{1}0]$. The corresponding position of the HM symbol is marked by 2, the other (empty) position is marked by 1: *P*321, *P*312, $P3_121$, $P3_112$ *etc. Note*: *P*321 and *P*312 denote *different* space-group types.

(3) In addition to the threefold axes, there are reflection planes or glide planes with their representative normals in the horizontal directions [100] or $[1\bar{1}0]$. The corresponding position of the HM symbol is marked by *m* or *c*, the empty position is marked by 1: *P*3*m*1 or *P*31*m etc.*

(4) The main axis in [001] is $\overline{3}$. Because $\overline{3}$ contains an inversion, the second or third position in the full HM symbol is marked by 2/*m* or 2/*c*, which leads to the HM symbols $P\,\overline{3}\,2/m\,1$ or

$P\bar{3}\,1\,2/m$ *etc.* In the short HM symbol the '2/' is not kept: $P\bar{3}m1$ or $P\bar{3}1m$ *etc.*

1.4.1.4.7.2. Hexagonal space groups

Hexagonal space groups have either one or three representative symmetry directions. The space groups of crystal classes 6, $\bar{6}$ and $6/m$ have [001] as their single symmetry direction for the axis 6 or 6_k for $k = 1, \ldots, 5$ or $\bar{6}$, and for the plane m with its normal along [001]. The short and full HM symbols are the same. Examples are $P6$, $P6_4$, $P\bar{6}$ and $P6_3/m$.

Space groups of crystal classes 622, $6mm$, $\bar{6}2m$ and $6/m\,2/m\,2/m$ have the representative symmetry directions [001], [100] and $[1\bar{1}0]$. As opposed to the trigonal HM symbols, in the hexagonal HM symbols no symmetry direction is 'empty' and occupied by '1'.

In space groups of the crystal classes 622, $6mm$ and $\bar{6}2m$ the short and full HM symbols are the same; in $6/m\,2/m\,2/m$ the short symbols are deprived of the parts '2/' of the full symbols. The full HM symbol $P\,6_3/m\,2/m\,2/c$ is shortened to the short HM symbol $P6_3/mmc$, the full HM symbol $P\,6_3/m\,2/c\,2/m$ is shortened to $P6_3/mcm$. The two denote different space-group types.

1.4.1.4.7.3. Rhombohedral space groups

The rhombohedral lattice may be understood as an R-centred hexagonal lattice and then referred to the hexagonal basis. It has two kinds of symmetry directions, which coincide with the primary and secondary symmetry directions of the hexagonal lattice (owing to the R centrings, no symmetry operation along the tertiary symmetry direction of the hexagonal lattice is compatible with the rhombohedral lattice). On the other hand, the rhombohedral lattice may be referred to a (primitive) rhombohedral coordinate system with the lattice parameters $a = b = c$ and $\alpha = \beta = \gamma$. The HM symbol of a rhombohedral space group starts with R, its representative symmetry directions are $[001]_{\rm hex}$ or $[111]_{\rm rhomb}$ and $[100]_{\rm hex}$ or $[1\bar{1}0]_{\rm rhomb}$. In this section the rhombohedral primitive cell is used. The rotations 3 and the rotoinversions $\bar{3}$ are accompanied by screw rotations 3_1 and 3_2. Rotations 2 about horizontal axes always alternate with 2_1 screw rotations and reflections m are accompanied by different glide reflections g with unconventional glide components. The additional operations mentioned are not listed in the full HM symbols.

The seven rhombohedral space groups belong to the five crystal classes 3, $\bar{3}$, 32, $3m$ and $\bar{3}2/m$. In $R3$ and $R\bar{3}$ only the first of the symmetry directions is occupied and listed in the full and short HM symbols. In the space groups of the other crystal classes the second symmetry direction $[1\bar{1}0]$ is occupied by '2' or 'm' or 'c' or '$2/m$' or '$2/c$', leading to the full HM symbols $R32$, $R3m$, $R3c$, $R\bar{3}2/m$ and $R\bar{3}2/c$. In the short HM symbols the '2/' parts of the last two symbols are skipped: $R\bar{3}m$ and $R\bar{3}c$.

1.4.1.4.8. Cubic space groups

There are five cubic crystal classes combined with the three types of lattices P, F and I in which the cubic space groups are classified. The two symmetry directions [100] and [111] are the representative directions in the space groups of the crystal classes 23 and $2/m\,\bar{3}$. A third representative symmetry direction, $[1\bar{1}0]$, is added for space groups of the crystal classes 432, $\bar{4}3m$ and $4/m\,\bar{3}\,2/m$.[6]

[6] Note: '3' or '$\bar{3}$' directly after the lattice symbol denotes a trigonal or rhombohedral space group; '3' or '$\bar{3}$' in the third position (second position after the lattice symbol) is characteristic for cubic space groups.

Table 1.4.1.2
The structure of the Hermann–Mauguin symbols for the plane groups

The positions of the representative symmetry directions for the crystal systems are given. The lattice symbol and the maximal order of rotations around a point are followed by two positions for symmetry directions.

Crystal system	Lattice(s)	First position	Second position	Third position
Oblique	p	1 or 2	—	—
Rectangular	p, c	1 or 2	**a**	**b**
Tetragonal	p	4	**a**	**a** − **b**
Hexagonal	p	3	**a**	1
			or	
		3	1	**a** − **b**
		6	**a**	**a** − **b**

In the full HM symbol the symmetry is described as usual. Examples are $P2_13$, $F\,2/d\,\bar{3}$, $P4_332$, $F\bar{4}3c$, $P\,4_2/m\,\bar{3}\,2/n$ and finally No. 230, $I\,4_1/a\,\bar{3}\,2/d$. The short HM symbols of the noncentrosymmetric space groups (those of crystal classes 23, 432 and $\bar{4}3m$) are the same as the full HM symbols. In the short HM symbols of centrosymmetric space groups of the crystal classes $2/m\,\bar{3}$ and $4/m\,\bar{3}\,2/m$ the rotations or screw rotations are omitted with the exception of the rotations 3 and rotoinversions $\bar{3}$ which represent the symmetry in direction [111]. Thus, in the examples listed above, $Fd\bar{3}$, $Pm\bar{3}n$ and $Ia\bar{3}d$ are the short HM symbols differing from the full HM symbols.

As in the orthorhombic space groups $I222$ and $I2_12_12_1$, there is the pair $I23$ and $I2_13$ in which the 'simplest symmetry operation' rule is violated. In both space groups twofold rotations and screw rotations around **a**, **b** and **c** occur simultaneously. In $I23$ the rotation axes intersect, in $I2_13$ they do not. The first space group can be generated by adding the I-centring to the space group $P23$, the second is obtained by adding the I-centring to the space group $P2_13$.

1.4.1.5. Hermann–Mauguin symbols of the plane groups

The principles of the HM symbols for space groups are retained in the HM symbols for plane groups (also known as *wallpaper groups*). The rotation axes along **c** of three dimensions are replaced by *rotation points* in the **ab** plane; the possible orders of rotations are the same as in three-dimensional space: 2, 3, 4 and 6. The lattice (sometimes called *net*) of a plane group is spanned by the two basis vectors **a** and **b**, and is designated by a lower-case letter. The choice of a lattice basis, *i.e.* of a minimal cell, leads to a primitive lattice p, in addition a c-centred lattice is conventionally used. The nets are listed in Table 3.1.2.1. The reflections and glide reflections through planes of the space groups are replaced by *reflections and glide reflections through lines*. Glide reflections are called g independent of the direction of the glide line. The arrangement of the constituents in the HM symbol is displayed in Table 1.4.1.2.

Short HM symbols are used only if there is at most one symmetry direction, *e.g.* $p411$ is replaced by $p4$ (no symmetry direction), $p1m1$ is replaced by pm (one symmetry direction) *etc.*

There are four crystal systems of plane groups, *cf.* Table 3.2.3.1. The analogue of the triclinic crystal system is called *oblique*, the analogues of the monoclinic and orthorhombic crystal systems are *rectangular*. Both have rotations of order 2 at most. The presence of reflection or glide reflection lines in the rectangular crystal system allows one to choose a rectangular basis with one basis vector perpendicular to a symmetry line and one basis

vector parallel to it. The *square* crystal system is analogous to the tetragonal crystal system for space groups by the occurrence of fourfold rotation points and a square net. Plane groups with threefold and sixfold rotation points are united in the *hexagonal* crystal system with a hexagonal net.

Plane groups occur as sections and projections of the space groups, *cf.* Section 1.4.5. In order to maintain the relations to the space groups, the symmetry directions of the symmetry lines are determined by their normals, not by the directions of the lines themselves. This is important because the normal of the line, not the direction of the line itself, determines the position in the HM symbol.

(1) In oblique plane groups there is no symmetry direction: HM symbols are $p1$ or $p2$.

(2) Rectangular plane groups may have no rotations and then only one symmetry direction: $p1m1 = pm$, $p1g1 = pg$ and $c1m1 = cm$. If there are twofold rotations, the HM symbol starts with $p2$ or $c2$, followed by the symmetry m or g first perpendicular to **a** and then perpendicular to **b**. The conventional HM symbol $p2mg$ describes a plane group with a reflection line running perpendicular to **a** (parallel to **b**) and a glide-reflection line running from the back to the front (perpendicular to **b** and thus parallel to **a**). There are four plane-group types: $p2mm$, $p2mg$, $p2gg$ and $c2mm$. The constituent '2' was sometimes omitted in older HM symbols.

(3) There is one square plane group with only rotations and no symmetry directions, the net is a square net: $p411 = p4$. The generating symmetry of symmetry directions perpendicular to **a** and **a** − **b** are listed in the second and third positions: $p4mm$ with reflection lines perpendicular to **a** and **b** and $p4gm$ with glide lines in the same directions. Reflection lines and glide lines perpendicular to **a** − **b** (and **a** + **b**) alternate.

(4) Five plane groups belong to the hexagonal crystal system. The trigonal and hexagonal plane groups $p311 = p3$ and $p611 = p6$ contain only rotations. In the other trigonal plane groups there is exactly one set of symmetry directions; its representative direction is either perpendicular to **a** ($p3m1$) or perpendicular to **a** − **b** ($p31m$).

The HM symbols $p3m1$ and $p31m$ may be easily confused, although they are different. Apart from the different orientations of their symmetry directions, in a plane group of type $p3m1$, all rotation points lie on reflection lines, but in $p31m$ not all of them do.

The hexagonal plane group $p6mm$ displays representative directions of mirror lines perpendicular to **a** *and* perpendicular to **a** − **b**.

1.4.1.6. Sequence of space-group types

The sequence of space-group entries in the space-group tables follows that introduced by Schoenflies (1891) and is thus established historically. Within each geometric crystal class, Schoenflies numbered the space-group types in an obscure way. As early as 1919, Niggli (1919) considered this Schoenflies sequence to be unsatisfactory and suggested that another sequence might be more appropriate. Fedorov (1891) used a different sequence in order to distinguish between symmorphic, hemisymmorphic and asymmorphic space groups (*cf.* Section 1.3.3.3 for a detailed discussion of symmorphic space groups).

The basis of the Schoenflies symbols and thus of the Schoenflies listing is the geometric crystal class. For the present space-group tables, a sequence might have been preferred in which, in addition, space-group types belonging to the same arithmetic crystal class were grouped together. It was decided, however, that the long-established sequence in the earlier editions of *International Tables* should not be changed.

In Table 1.4.1.3, those geometric crystal classes are listed in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class (*cf.* Section 1.3.4.4 for the definition and discussion of arithmetic crystal classes). The space

Table 1.4.1.3
List of geometric crystal classes in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class

Geometric crystal class	Space-group type		
	No.	Hermann–Mauguin symbol	Schoenflies symbol
$2/m$	10	$P2/m$	C_{2h}^1
	11	$P2_1/m$	C_{2h}^2
	13	$P2/c$	C_{2h}^4
	14	$P2_1/c$	C_{2h}^5
	12	$C2/m$	C_{2h}^3
	15	$C2/c$	C_{2h}^6
32	149	$P312$	D_3^1
	151	$P3_112$	D_3^3
	153	$P3_212$	D_3^5
	150	$P321$	D_3^2
	152	$P3_121$	D_3^4
	154	$P3_221$	D_3^6
	155	$R32$	D_3^7
$3m$	156	$P3m1$	C_{3v}^1
	158	$P3c1$	C_{3v}^3
	157	$P31m$	C_{3v}^2
	159	$P31c$	C_{3v}^4
	160	$R3m$	C_{3v}^5
	161	$R3c$	C_{3v}^6
23	195	$P23$	T^1
	198	$P2_13$	T^4
	196	$F23$	T^2
	197	$I23$	T^3
	199	$I2_13$	T^5
$m\bar{3}$	200	$Pm\bar{3}$	T_h^1
	201	$Pn\bar{3}$	T_h^2
	205	$Pa\bar{3}$	T_h^6
	202	$Fm\bar{3}$	T_h^3
	203	$Fd\bar{3}$	T_h^4
	204	$Im\bar{3}$	T_h^5
	206	$Ia\bar{3}$	T_h^7
432	207	$P432$	O^1
	208	$P4_232$	O^2
	213	$P4_132$	O^7
	212	$P4_332$	O^6
	209	$F432$	O^3
	210	$F4_132$	O^4
	211	$I432$	O^5
	214	$I4_132$	O^8
$\bar{4}3m$	215	$P\bar{4}3m$	T_d^1
	218	$P\bar{4}3n$	T_d^4
	216	$F\bar{4}3m$	T_d^2
	219	$F\bar{4}3c$	T_d^5
	217	$I\bar{4}3m$	T_d^3
	220	$I\bar{4}3d$	T_d^6

groups are rearranged in such a way that space groups of the same arithmetic crystal class are grouped together. The arithmetic crystal classes are separated by rules spanning the last three columns of the table and the geometric crystal classes are separated by rules spanning the full width of the table. In all cases not listed in Table 1.4.1.3, the Schoenflies sequence, as used in the space-group tables, does not break up arithmetic crystal classes. Nevertheless, some rearrangement would be desirable in other arithmetic crystal classes too. For example, the symmorphic space group should always be the first entry of each arithmetic crystal class.

1.4.2. Descriptions of space-group symmetry operations

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

One of the aims of the space-group tables of Chapter 2.3 is to represent the symmetry operations of each of the 17 plane groups and 230 space groups. The following sections offer a short description of the symbols of the symmetry operations, their listings and their graphical representations as found in the space-group tables of Chapter 2.3. For a detailed discussion of crystallographic symmetry operations and their matrix–column presentation $(\boldsymbol{W}, \boldsymbol{w})$ the reader is referred to Chapter 1.2.

1.4.2.1. Symbols for symmetry operations

Given the analytical description of the symmetry operations by matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$, their geometric meaning can be determined following the procedure discussed in Section 1.2.2. The notation scheme of the symmetry operations applied in the space-group tables was designed by W. Fischer and E. Koch, and the following description of the symbols partly reproduces the explanations by the authors given in Section 11.1.2 of *IT* A5. Further explanations of the symbolism and examples are presented in Section 2.1.3.9.

The symbol of a symmetry operation indicates the type of the operation, its screw or glide component (if relevant) and the location of the corresponding geometric element (*cf.* Section 1.2.3 and Table 1.2.3.1 for a discussion of geometric elements). The symbols of the symmetry operations explained below are based on the Hermann–Mauguin symbols (*cf.* Section 1.4.1.4), modified and supplemented where necessary.

The symbol for the *identity* mapping is 1.

A *translation* is symbolized by the letter t followed by the components of the translation vector between parentheses. *Example*: $t(\frac{1}{2}, \frac{1}{2}, 0)$ represents a translation by a vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, *i.e.* a C centring.

A *rotation* is symbolized by a number $n = 2, 3, 4$ or 6 (according to the rotation angle $360^\circ/n$) and a superscript + or −, which specifies the sense of rotation ($n > 2$). The symbol of rotation is followed by the location of the rotation axis. *Example*: $4^+\ 0, y, 0$ indicates a rotation of 90° about the line $0, y, 0$ that brings point $0, 0, 1$ onto point $1, 0, 0$, *i.e.* a counter-clockwise rotation (or rotation in the mathematically *positive sense*) if viewed from point $0, 1, 0$ to point $0, 0, 0$.

A *screw rotation* is symbolized in the same way as a pure rotation, but with the screw part added between parentheses. *Example*: $3^-(0, 0, \frac{1}{3})\ \frac{2}{3}, \frac{1}{3}, z$ indicates a clockwise rotation of 120° around the line $\frac{2}{3}, \frac{1}{3}, z$ (or rotation in the mathematically *negative sense*) if viewed from the point $\frac{2}{3}, \frac{1}{3}, 1$ towards $\frac{2}{3}, \frac{1}{3}, 0$, combined with a translation of $\frac{1}{3}\mathbf{c}$.

A *reflection* is symbolized by the letter m, followed by the location of the mirror plane.

A *glide reflection* in general is symbolized by the letter g, with the glide part given between parentheses, followed by the location of the glide plane. These specifications characterize every glide reflection uniquely. Exceptions are the traditional symbols a, b, c, n and d that are used instead of g. In the case of a glide plane a, b or c, the explicit statement of the glide vector is omitted if it is $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$ or $\frac{1}{2}\mathbf{c}$, respectively. *Examples*: $a\ x, y, \frac{1}{4}$ means a glide reflection with glide vector $\frac{1}{2}\mathbf{a}$ and through a plane $x, y, \frac{1}{4}$; $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})\ x, x - \frac{1}{4}, z$ denotes a glide reflection with glide part $(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ and the glide plane d at $x, x - \frac{1}{4}, z$.

An *inversion* is symbolized by $\bar{1}$ followed by the location of the inversion centre.

A *rotoinversion* is symbolized, in analogy with a rotation, by $\bar{3}$, $\bar{4}$ or $\bar{6}$ and the superscript + or −, again followed by the location of the (rotoinversion) axis. Note that angle and sense of rotation refer to the pure rotation and not to the combination of rotation and inversion. In addition, the location of the inversion point is given by the appropriate coordinate triplet after a semicolon. *Example*: $\bar{4}^+\ 0, \frac{1}{2}, z; 0, \frac{1}{2}, \frac{1}{4}$ means a 90° rotoinversion with axis at $0, \frac{1}{2}, z$ and inversion point at $0, \frac{1}{2}, \frac{1}{4}$. The rotation is performed in the mathematically positive sense when viewed from $0, \frac{1}{2}, 1$ towards $0, \frac{1}{2}, 0$. Therefore, the rotoinversion maps point $0, 0, 0$ onto point $-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

The notation scheme is extensively applied in the symmetry-operations blocks of the space-group descriptions in the tables of Chapter 2.3. The numbering of the entries of the symmetry-operations block corresponds to that of the coordinate triplets of the general position, and in space groups with primitive cells the two lists contain the same number of entries. As an example consider the symmetry-operations block of the space group $P2_1/c$ shown in Fig. 1.4.2.1. The four entries correspond to the four coordinate triplets of the general-position block of the group and provide the geometric description of the symmetry operations chosen as

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$ (3) $\bar{1}\ \ 0,0,0$ (4) $c\ \ x,\frac{1}{4},z$

Figure 1.4.2.1
General-position and symmetry-operations blocks for the space group $P2_1/c$, No. 14 (unique axis b, cell choice 1). The coordinate triplets of the general position, numbered from (1) to (4), correspond to the four coset representatives of the decomposition of $P2_1/c$ with respect to its translation subgroup, *cf.* Table 1.4.2.6. The entries of the symmetry-operations block numbered from (1) to (4) describe geometrically the symmetry operations represented by the four coordinate triplets of the general-position block.