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1.4. Space groups and their descriptions

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1.4.1. Symbols of space groups

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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

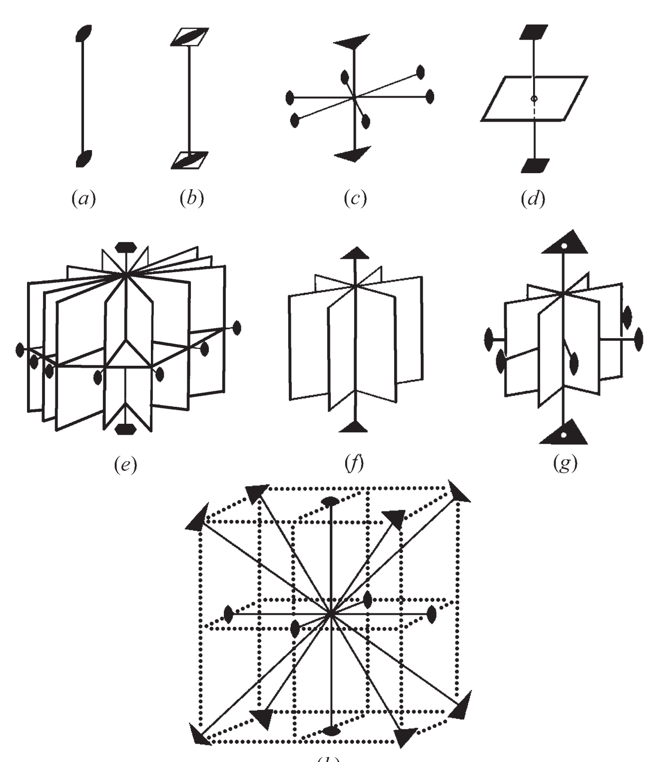

Figure 1.4.1.1
Symmetry-element diagrams of some point groups [adapted from Vainshtein (1994)]. The point groups are specified by their Schoenflies and Hermann–Mauguin symbols. (*a*) $C_2 = 2$, (*b*) $S_4 = \bar{4}$, (*c*) $D_3 = 32$, (*d*) $C_{4h} = 4/m$, (*e*) $D_{6h} = 6/m\,2/m\,2/m$, (*f*) $C_{3v} = 3m$, (*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 $P121$, but they may also include several symmetry operations, *e.g.* 2, 2_1, m and a in space group $C12/m1$. 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 $C12/m1$ 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 ⟨$\bar{1}\bar{1}\bar{1}$⟩ 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) $P\bar{1}$, $P12/c1$, $A112/m$, $F2/d\,2/d\,2/d$, $I4_1/a$, $P\,4/m\,2_1/n\,2/c$, $P\bar{3}$, $P3m1$, $P3_112$, $R\bar{3}2/c$, $P6_3/m$, $P6_122$ 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 $P\,2/m\,2/n\,2_1/a$ may appear as $P\,2/n\,2/m\,2_1/b$ or $P\,2/n\,2_1/c\,2/m$ or $P\,2_1/c\,2/n\,2/m$ or $P\,2_1/b\,2/m\,2/n$ or $P\,2/m\,2_1/a\,2/n$ 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 $P\,2_1/b\,2_1/a\,2/m \rightarrow 2/m\,2/m\,2/m$ 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. $P1m1$ or $P11m$ may designate the same space group but in different settings. $Pm11$ 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: $P2$, $P2_1$, $C2$, Pm, Pc, Cm, Cc, $P2/m$, $P2_1/m$, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$. 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, $mm2$ 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 $mm2$ 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 $P222$, $P222_1$, $P2_12_12$ 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 $mm2$ 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 $mm2$ 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, $Pmm2$, $Pmc2_1$, $Pba2$ 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, $P2/m\,2/m\,2/m$, $P2_1/m\,2/m\,2/a$, $P2/m\,2/n\,2_1/a$, $P2_1/b\,2_1/a\,2/m$ 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 $P222$, 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 $I222$, but only the space group generated from $P222$ is named $I222$, 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 $mm2$ 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, $\bar{4}$ and 4/*m* have only one symmetry direction, [001]. The other four classes, 422, 4*mm*, $\bar{4}2m$ 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 $\bar{4}$ these are rotoinversion axes $\bar{4}$; 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 $\bar{4}$ 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 [$\bar{1}\bar{1}0$] (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 $\bar{4}$ persists. Full HM symbols of space groups are, among others, $P4_22_12$, $P4_2bc$, $P\bar{4}2c$ 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 $\bar{4}2m$. 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 $\bar{3}$. The short and the full HM symbols are *P*3, $P3_1$, $P3_2$, $P\bar{3}$.

(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 $\bar{3}$. Because $\bar{3}$ 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 $P\,\bar{3}\,2/m\,1$ 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 *P*6, $P6_4$, $P\bar{6}$ and $P6_3/m$.

Space groups of crystal classes 622, 6*mm*, $\bar{6}2m$ 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, 6*mm* 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, 3*m* and $\bar{3}2/m$. In *R*3 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 *R*32, *R*3*m*, *R*3*c*, $R\bar{3}2/m$ 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 *I*222 and $I2_12_12_1$, there is the pair *I*23 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 *I*23 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 *P*23, 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.* *p*411 is replaced by *p*4 (no symmetry direction), *p*1*m*1 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 $360°/n$) 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.

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
16 *e* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$

Symmetry operations

For $(0,0,0)+$ set			
(1) 1	(2) 2 $0,0,z$	(3) m $x,0,z$	(4) m $0,y,z$
For $(0,\frac{1}{2},\frac{1}{2})+$ set			
(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) c $x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
For $(\frac{1}{2},0,\frac{1}{2})+$ set			
(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(4) c $\frac{1}{4},y,z$
For $(\frac{1}{2},\frac{1}{2},0)+$ set			
(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) a $x,\frac{1}{4},z$	(4) b $\frac{1}{4},y,z$

Figure 1.4.2.2

General-position and symmetry-operations blocks as given in the space-group tables for space group *Fmm*2 (42). The numbering scheme of the entries in the different symmetry-operations blocks follows that of the general position.

coset representatives of $P2_1/c$ with respect to its translation subgroup.

For space groups with conventional *centred* cells, there are several (2, 3 or 4) blocks of symmetry operations: one block for each of the translations listed below the subheading 'Coordinates'. Consider, for example, the four symmetry-operations blocks of the space group *Fmm*2 (42) reproduced in Fig. 1.4.2.2. They correspond to the four sets of coordinate triplets of the general position obtained by the translations $t(0, 0, 0)$, $t(0, \frac{1}{2}, \frac{1}{2})$, $t(\frac{1}{2}, 0, \frac{1}{2})$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$, *cf.* Fig. 1.4.2.2. The numbering scheme of the entries in the different symmetry-operations blocks follows that of the general position. For example, the geometric description of entry (4) in the symmetry-operations block under the heading 'For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set' of *Fmm*2 corresponds to the coordinate triplet $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, z$, which is obtained by adding $t(\frac{1}{2}, \frac{1}{2}, 0)$ to the translation part of the printed coordinate triplet (4) $\bar{x}, y, z$ (*cf.* Fig. 1.4.2.2).

1.4.2.2. Seitz symbols of symmetry operations

Apart from the notation for the geometric interpretation of the matrix–column representation of symmetry operations $(\boldsymbol{W}, \boldsymbol{w})$ discussed in detail in the previous section, there is another notation which has been adopted and is widely used by solid-state physicists and chemists. This is the so-called Seitz notation $\{\boldsymbol{R}|\boldsymbol{v}\}$ introduced by Seitz in a series of papers on the matrix-algebraic development of crystallographic groups (Seitz, 1935).

Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ reflect the fact that space-group operations are affine mappings and are essentially shorthand descriptions of the matrix–column representations of the symmetry operations of the space groups. They consist of two parts: a rotation (or linear) part $\boldsymbol{R}$ and a translation part $\boldsymbol{v}$. The Seitz symbol is specified between braces and the rotational and the translational parts are separated by a vertical line. The translation parts $\boldsymbol{v}$ correspond exactly to the columns $\boldsymbol{w}$ of the coordinate triplets of the general-position blocks of the space-group tables. The rotation parts $\boldsymbol{R}$ consist of symbols that specify (i) the type and the order of the symmetry operation, and (ii) the orientation of the corresponding symmetry element with respect to the basis. The orientation is denoted by the direction of the axis for rotations or rotoinversions, or the direction of the normal to reflection planes. (Note that in the latter case this is different from the way the orientation of reflection planes is given in the symmetry-operations block.)

The linear parts of Seitz symbols are denoted in many different ways in the literature (Litvin & Kopsky, 2011). According to the conventions approved by the Commission of Crystallographic Nomenclature of the International Union of Crystallography (Glazer *et al.*, 2014) the symbol $\boldsymbol{R}$ is 1 and $\bar{1}$ for the identity and the inversion, m for reflections, the symbols 2, 3, 4 and 6 are used for rotations and $\bar{3}$, $\bar{4}$ and $\bar{6}$ for rotoinversions. For rotations and rotoinversions of order higher than 2, a superscript + or − is used to indicate the sense of the rotation. Subscripts of the symbols $\boldsymbol{R}$ denote the characteristic direction of the operation: for example, the subscripts 100, 010 and $1\bar{1}0$ refer to the directions [100], [010] and $[1\bar{1}0]$, respectively.

Examples

(*a*) Consider the coordinate triplets of the general positions of $P2_12_12$ (18):

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

The corresponding geometric interpretations of the symmetry operations are given by

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

In Seitz notation the symmetry operations are denoted by

(1) $\{1|0\}$ (2) $\{2_{001}|0\}$ (3) $\{2_{010}|\frac{1}{2}, \frac{1}{2}, 0\}$ (4) $\{2_{100}|\frac{1}{2}, \frac{1}{2}, 0\}$

(*b*) Similarly, the symmetry operations corresponding to the general-position coordinate triplets of $P2_1/c$ (14), *cf.* Fig. 1.4.2.1, in Seitz notation are given as

(1) $\{1|0\}$ (2) $\{2_{010}|0, \frac{1}{2}, \frac{1}{2}\}$ (3) $\{\bar{1}|0\}$ (4) $\{m_{010}|0, \frac{1}{2}, \frac{1}{2}\}$

The linear parts $\boldsymbol{R}$ of the Seitz symbols of the space-group symmetry operations are shown in Tables 1.4.2.1–1.4.2.3. Each symbol $\boldsymbol{R}$ is specified by the shorthand notation of its (3×3) matrix representation (also known as the *Jones' faithful representation symbol*, *cf.* Bradley & Cracknell, 1972), the type of symmetry operation and its orientation as described in the corresponding symmetry-operations block of the space-group tables of this volume. The sequence of $\boldsymbol{R}$ symbols in Table 1.4.2.1 corresponds to the numbering scheme of the general-position coordinate triplets of the space groups of the $m\bar{3}m$ crystal class, while those of Table 1.4.2.2 and Table 1.4.2.3 correspond to the general-position sequences of the space groups of $6/mmm$ and $\bar{3}m$ (rhombohedral axes) crystal classes, respectively.

The same symbols $\boldsymbol{R}$ can be used for the construction of Seitz symbols for the symmetry operations of subperiodic layer and rod groups (Litvin & Kopsky, 2014), and magnetic groups, or for the designation of the symmetry operations of the point groups of space groups. [One should note that the Seitz symbols applied in

Table 1.4.2.1
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for space-group symmetry operations of cubic, tetragonal, orthorhombic, monoclinic and triclinic crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	x, y, z	1		1
2	$\bar{x}, \bar{y}, z$	2	$0, 0, z$	2_{001}
3	$\bar{x}, y, \bar{z}$	2	$0, y, 0$	2_{010}
4	$x, \bar{y}, \bar{z}$	2	$x, 0, 0$	2_{100}
5	z, x, y	3^{+}	x, x, x	3^{+}_{111}
6	$z, \bar{x}, \bar{y}$	3^{+}	$\bar{x}, x, \bar{x}$	$3^{+}_{\bar{1}1\bar{1}}$
7	$\bar{z}, \bar{x}, y$	3^{+}	$x, \bar{x}, \bar{x}$	$3^{+}_{1\bar{1}\bar{1}}$
8	$\bar{z}, x, \bar{y}$	3^{+}	$\bar{x}, \bar{x}, x$	$3^{+}_{\bar{1}\bar{1}1}$
9	y, z, x	3^{-}	x, x, x	3^{-}_{111}
10	$\bar{y}, z, \bar{x}$	3^{-}	$x, \bar{x}, \bar{x}$	$3^{-}_{1\bar{1}\bar{1}}$
11	$y, \bar{z}, \bar{x}$	3^{-}	$\bar{x}, \bar{x}, x$	$3^{-}_{\bar{1}\bar{1}1}$
12	$\bar{y}, \bar{z}, x$	3^{-}	$\bar{x}, x, \bar{x}$	$3^{-}_{\bar{1}1\bar{1}}$
13	$y, x, \bar{z}$	2	$x, x, 0$	2_{110}
14	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
15	$y, \bar{x}, z$	4^{-}	$0, 0, z$	4^{-}_{001}
16	$\bar{y}, x, z$	4^{+}	$0, 0, z$	4^{+}_{001}
17	$x, z, \bar{y}$	4^{-}	$x, 0, 0$	4^{-}_{100}
18	$\bar{x}, z, y$	2	$0, y, y$	2_{011}
19	$\bar{x}, \bar{z}, \bar{y}$	2	$0, y, \bar{y}$	$2_{01\bar{1}}$
20	$x, \bar{z}, y$	4^{+}	$x, 0, 0$	4^{+}_{100}
21	$z, y, \bar{x}$	4^{+}	$0, y, 0$	4^{+}_{010}
22	$z, \bar{y}, x$	2	$x, 0, x$	2_{101}
23	$\bar{z}, y, x$	4^{-}	$0, y, 0$	4^{-}_{010}
24	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
25	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
26	$x, y, \bar{z}$	m	$x, y, 0$	m_{001}
27	$x, \bar{y}, z$	m	$x, 0, z$	m_{010}
28	$\bar{x}, y, z$	m	$0, y, z$	m_{100}
29	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^{+}$	x, x, x	$\bar{3}^{+}_{111}$
30	$\bar{z}, x, y$	$\bar{3}^{+}$	$\bar{x}, x, \bar{x}$	$\bar{3}^{+}_{\bar{1}1\bar{1}}$
31	$z, x, \bar{y}$	$\bar{3}^{+}$	$x, \bar{x}, \bar{x}$	$\bar{3}^{+}_{1\bar{1}\bar{1}}$
32	$z, \bar{x}, y$	$\bar{3}^{+}$	$\bar{x}, \bar{x}, x$	$\bar{3}^{+}_{\bar{1}\bar{1}1}$
33	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^{-}$	x, x, x	$\bar{3}^{-}_{111}$
34	$y, \bar{z}, x$	$\bar{3}^{-}$	$x, \bar{x}, \bar{x}$	$\bar{3}^{-}_{1\bar{1}\bar{1}}$
35	$\bar{y}, z, x$	$\bar{3}^{-}$	$\bar{x}, \bar{x}, x$	$\bar{3}^{-}_{\bar{1}\bar{1}1}$
36	$y, z, \bar{x}$	$\bar{3}^{-}$	$\bar{x}, x, \bar{x}$	$\bar{3}^{-}_{\bar{1}1\bar{1}}$
37	$\bar{y}, \bar{x}, z$	m	$x, \bar{x}, z$	m_{110}
38	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
39	$\bar{y}, x, \bar{z}$	$\bar{4}^{-}$	$0, 0, z$	$\bar{4}^{-}_{001}$
40	$y, \bar{x}, \bar{z}$	$\bar{4}^{+}$	$0, 0, z$	$\bar{4}^{+}_{001}$
41	$\bar{x}, \bar{z}, y$	$\bar{4}^{-}$	$x, 0, 0$	$\bar{4}^{-}_{100}$
42	$x, \bar{z}, \bar{y}$	m	$x, y, \bar{y}$	m_{011}
43	x, z, y	m	x, y, y	$m_{01\bar{1}}$
44	$\bar{x}, z, \bar{y}$	$\bar{4}^{+}$	$x, 0, 0$	$\bar{4}^{+}_{100}$
45	$\bar{z}, \bar{y}, x$	$\bar{4}^{+}$	$0, y, 0$	$\bar{4}^{+}_{010}$
46	$\bar{z}, y, \bar{x}$	m	$\bar{x}, y, x$	m_{101}
47	$z, \bar{y}, \bar{x}$	$\bar{4}^{-}$	$0, y, 0$	$\bar{4}^{-}_{010}$
48	z, y, x	m	x, y, x	$m_{\bar{1}01}$

Table 1.4.2.2
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for space-group symmetry operations of hexagonal and trigonal crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	x, y, z	1		1
2	$\bar{y}, x-y, z$	3^{+}	$0, 0, z$	3^{+}_{001}
3	$\bar{x}+y, \bar{x}, z$	3^{-}	$0, 0, z$	3^{-}_{001}
4	$\bar{x}, \bar{y}, z$	2	$0, 0, z$	2_{001}
5	$y, \bar{x}+y, z$	6^{-}	$0, 0, z$	6^{-}_{001}
6	$x-y, x, z$	6^{+}	$0, 0, z$	6^{+}_{001}
7	$y, x, \bar{z}$	2	$x, x, 0$	2_{110}
8	$x-y, \bar{y}, \bar{z}$	2	$x, 0, 0$	2_{100}
9	$\bar{x}, \bar{x}+y, \bar{z}$	2	$0, y, 0$	2_{010}
10	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
11	$\bar{x}+y, y, \bar{z}$	2	$x, 2x, 0$	2_{120}
12	$x, x-y, \bar{z}$	2	$2x, x, 0$	2_{210}
13	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
14	$y, \bar{x}+y, \bar{z}$	$\bar{3}^{+}$	$0, 0, z$	$\bar{3}^{+}_{001}$
15	$x-y, x, \bar{z}$	$\bar{3}^{-}$	$0, 0, z$	$\bar{3}^{-}_{001}$
16	$x, y, \bar{z}$	m	$x, y, 0$	m_{001}
17	$\bar{y}, x-y, \bar{z}$	$\bar{6}^{-}$	$0, 0, z$	$\bar{6}^{-}_{001}$
18	$\bar{x}+y, \bar{x}, \bar{z}$	$\bar{6}^{+}$	$0, 0, z$	$\bar{6}^{+}_{001}$
19	$\bar{y}, \bar{x}, z$	m	$x, \bar{x}, z$	m_{110}
20	$\bar{x}+y, y, z$	m	$x, 2x, z$	m_{100}
21	$x, x-y, z$	m	$2x, x, z$	m_{010}
22	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
23	$x-y, \bar{y}, z$	m	$x, 0, z$	m_{120}
24	$\bar{x}, \bar{x}+y, z$	m	$0, y, z$	m_{210}

Table 1.4.2.3
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for symmetry operations of rhombohedral space groups (rhombohedral-axes setting)

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	x, y, z	1		1
2	z, x, y	3^{+}	x, x, x	3^{+}_{111}
3	y, z, x	3^{-}	x, x, x	3^{-}_{111}
4	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
5	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
6	$\bar{x}, \bar{z}, \bar{y}$	2	$0, y, \bar{y}$	$2_{01\bar{1}}$
7	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
8	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^{+}$	x, x, x	$\bar{3}^{+}_{111}$
9	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^{-}$	x, x, x	$\bar{3}^{-}_{111}$
10	z, y, x	m	x, y, x	$m_{\bar{1}01}$
11	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
12	x, z, y	m	x, y, y	$m_{01\bar{1}}$

Table 1.4.2.4
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for plane-group symmetry operations of oblique, rectangular and square crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction (if applicable).

IT A description				Seitz symbol
No.	Coordinate doublet	Type	Orientation	
1	x, y	1		1
2	$\bar{x}, \bar{y}$	2		2
3	$\bar{y}, x$	4^+		4^+
4	$y, \bar{x}$	4^-		4^-
5	$\bar{x}, y$	m	$0, y$	m_{10}
6	$x, \bar{y}$	m	$x, 0$	m_{01}
7	y, x	m	x, x	$m_{1\bar{1}}$
8	$\bar{y}, \bar{x}$	m	$x, \bar{x}$	m_{11}

Table 1.4.2.5
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for plane-group symmetry operations of the hexagonal crystal system

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction (if applicable).

IT A description				Seitz symbol
No.	Coordinate doublet	Type	Orientation	
1	x, y	1		1
2	$\bar{y}, x - y$	3^+		3^+
3	$\bar{x} + y, \bar{x}$	3^-		3^-
4	$\bar{x}, \bar{y}$	2		2
5	$y, \bar{x} + y$	6^-		6^-
6	$x - y, x$	6^+		6^+
7	$\bar{y}, \bar{x}$	m	$x, \bar{x}$	m_{11}
8	$\bar{x} + y, y$	m	$x, 2x$	m_{10}
9	$x, x - y$	m	$2x, x$	m_{01}
10	y, x	m	x, x	$m_{1\bar{1}}$
11	$x - y, \bar{y}$	m	$x, 0$	m_{12}
12	$\bar{x}, \bar{x} + y$	m	$0, y$	m_{21}

the first and second editions of *IT* E and in the IUCr e-book on magnetic groups (Litvin, 2012) differ from the standard symbols adopted by the Commission of Crystallographic Nomenclature.]

The Seitz symbols for plane groups are constructed following similar rules to those for space groups. The rotation part $\boldsymbol{R}$ is 1 for the identity, m for reflections, and 2, 3, 4 and 6 are used for rotations. The orientation of a reflection line is specified by a subscript indicating the direction of its 'normal'. Obviously, the direction indicators are of no relevance for the rotation points. The linear parts $\boldsymbol{R}$ of the Seitz symbols of the plane-group symmetry operations are shown in Tables 1.4.2.4 and 1.4.2.5. Each symbol $\boldsymbol{R}$ is specified by the shorthand notation of its (2×2) matrix representation, the type of symmetry operation and, if applicable, its orientation as described in the corresponding symmetry-operations block of the plane-group tables of this volume. The sequence of $\boldsymbol{R}$ symbols in Table 1.4.2.4 corresponds to the numbering scheme of the general-position coordinate doublets of the plane group $p4mm$, while those of Table 1.4.2.5 correspond to the general-position sequence of the plane group $p6mm$. The same symbols $\boldsymbol{R}$ can be used for the construction of Seitz symbols for the symmetry operations of subperiodic frieze groups (Litvin & Kopsky, 2014).

As illustrated in the examples above, zero translations are normally specified by a single zero in the Seitz symbols, but in cases where it is unclear whether the symbol refers to a space- or a plane-group symmetry operation, an explicit indication of the components of the translation vector is recommended.

From the description given above, it is clear that Seitz symbols can be considered as shorthand modifications of the matrix–column presentation $(\boldsymbol{W}, \boldsymbol{w})$ of symmetry operations discussed in detail in Chapter 1.2: the translation parts of $\{\boldsymbol{R}|\boldsymbol{v}\}$ and $(\boldsymbol{W}, \boldsymbol{w})$ coincide, while the different (3×3) matrices $\boldsymbol{W}$ are represented by the symbols $\boldsymbol{R}$ shown in Tables 1.4.2.1–1.4.2.3. As a result, the expressions for the product and the inverse of symmetry operations in Seitz notation are rather similar to those of the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ discussed in detail in Chapter 1.2:

(*a*) product of symmetry operations:

$$\{\boldsymbol{R}_1|\boldsymbol{v}_1\}\{\boldsymbol{R}_2|\boldsymbol{v}_2\} = \{\boldsymbol{R}_1\boldsymbol{R}_2|\boldsymbol{R}_1\boldsymbol{v}_2 + \boldsymbol{v}_1\};$$

(*b*) inverse of a symmetry operation:

$$\{\boldsymbol{R}|\boldsymbol{v}\}^{-1} = \{\boldsymbol{R}^{-1}| - \boldsymbol{R}^{-1}\boldsymbol{v}\}.$$

Similarly, the action of a symmetry operation $\{\boldsymbol{R}|\boldsymbol{v}\}$ on the column of point coordinates $\boldsymbol{x}$ is given by $\{\boldsymbol{R}|\boldsymbol{v}\}\boldsymbol{x} = \boldsymbol{R}\boldsymbol{x} + \boldsymbol{v}$ [*cf.* Chapter 1.2, equation (1.2.2.4)].

The rotation parts of the Seitz symbols partly resemble the geometric-description symbols of symmetry operations described in Section 1.4.2.1 and listed in the symmetry-operation blocks of the space-group tables of this volume: $\boldsymbol{R}$ contains the information on the type and order of the symmetry operation, and its characteristic direction. The Seitz symbols do not *directly* indicate the location of the symmetry operation, nor its glide or screw component, if any.

1.4.2.3. Symmetry operations and the general position

The classifications of space groups introduced in Chapter 1.3 allow one to reduce the practically unlimited number of possible space groups to a finite number of space-group types. However, each individual space-group type still consists of an infinite number of symmetry operations generated by the set of all translations of the space group. A practical way to represent the symmetry operations of space groups is based on the coset decomposition of a space group with respect to its translation subgroup, which was introduced and discussed in Section 1.3.3.2. For our further considerations, it is important to note that the listings of the general position in the space-group tables can be interpreted in two ways:

(i) Each of the numbered entries lists the coordinate triplets of an image point of a starting point with coordinates x, y, z under a symmetry operation of the space group. This feature of the general position will be discussed in detail in Section 1.4.4.

(ii) Each of the numbered entries of the general position lists a symmetry operation of the space group by the shorthand notation of its matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ (*cf.* Section 1.2.2.1). This fact is not as obvious as the more 'crystallographic' aspect described under (i), but its importance becomes evident from the following discussion, where it is shown how to extract the full analytical symmetry information of space groups from the general-position data in the space-group tables of Chapter 2.3.

With reference to a conventional coordinate system, the set of symmetry operations $\{W\}$ of a space group $\mathcal{G}$ is described by the

Table 1.4.2.6
Right coset decomposition of space group $P2_1/c$, No. 14 (unique axis b, cell choice 1) with respect to the normal subgroup of translations $\mathcal{T}$

The numbers u_1, u_2 and u_3 are positive or negative integers.

x	y	z	$\bar{x}$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}$	$\bar{z}$	x	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
$x+1$	y	z	$\bar{x}+1$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}$	$\bar{z}$	$x+1$	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
$x+2$	y	z	$\bar{x}+2$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}$	$\bar{z}$	$x+2$	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
	⋮			⋮			⋮			⋮	
x	$y+1$	z	$\bar{x}$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}+1$	$\bar{z}$	x	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
$x+1$	$y+1$	z	$\bar{x}+1$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}+1$	$\bar{z}$	$x+1$	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
$x+2$	$y+1$	z	$\bar{x}+2$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}+1$	$\bar{z}$	$x+2$	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
	⋮			⋮			⋮			⋮	
x	$y+2$	z	$\bar{x}$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}+2$	$\bar{z}$	x	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
$x+1$	$y+2$	z	$\bar{x}+1$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}+2$	$\bar{z}$	$x+1$	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
$x+2$	$y+2$	z	$\bar{x}+2$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}+2$	$\bar{z}$	$x+2$	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
	⋮			⋮			⋮			⋮	
x	y	$z+1$	$\bar{x}$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}$	$\bar{y}$	$\bar{z}+1$	x	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
$x+1$	y	$z+1$	$\bar{x}+1$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+1$	$\bar{y}$	$\bar{z}+1$	$x+1$	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
$x+2$	y	$z+1$	$\bar{x}+2$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+2$	$\bar{y}$	$\bar{z}+1$	$x+2$	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
	⋮			⋮			⋮			⋮	
x	$y+1$	$z+1$	$\bar{x}$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}$	$\bar{y}+1$	$\bar{z}+1$	x	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
$x+1$	$y+1$	$z+1$	$\bar{x}+1$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+1$	$\bar{y}+1$	$\bar{z}+1$	$x+1$	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
$x+2$	$y+1$	$z+1$	$\bar{x}+2$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+2$	$\bar{y}+1$	$\bar{z}+1$	$x+2$	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
	⋮			⋮			⋮			⋮	
$x+u_1$	$y+u_2$	$z+u_3$	$\bar{x}+u_1$	$y+u_2+\frac{1}{2}$	$\bar{z}+u_3+\frac{1}{2}$	$\bar{x}+u_1$	$\bar{y}+u_2$	$\bar{z}+u_3$	$x+u_1$	$\bar{y}+u_2+\frac{1}{2}$	$z+u_3+\frac{1}{2}$
	⋮			⋮			⋮			⋮	

set of matrix–column pairs $\{(\boldsymbol{W}, \boldsymbol{w})\}$. The set $\mathcal{T}_{\mathcal{G}} = \{(\boldsymbol{I}, \boldsymbol{t})\}$ of all translations forms the *translation subgroup* $\mathcal{T}_{\mathcal{G}} \triangleleft \mathcal{G}$, which is a normal subgroup of $\mathcal{G}$ of finite index $[i]$. If $(\boldsymbol{W}, \boldsymbol{w})$ is a fixed symmetry operation, then all the products $\mathcal{T}_{\mathcal{G}}(\boldsymbol{W}, \boldsymbol{w}) = \{(\boldsymbol{I}, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w})\} = \{(\boldsymbol{W}, \boldsymbol{w}+\boldsymbol{t})\}$ of translations with $(\boldsymbol{W}, \boldsymbol{w})$ have the same rotation part $\boldsymbol{W}$. Conversely, every symmetry operation W of $\mathcal{G}$ with the same matrix part $\boldsymbol{W}$ is represented in the set $\mathcal{T}_{\mathcal{G}}(\boldsymbol{W}, \boldsymbol{w})$. The infinite set of symmetry operations $\mathcal{T}_{\mathcal{G}}(\boldsymbol{W}, \boldsymbol{w})$ is called a coset of the right coset decomposition of $\mathcal{G}$ with respect to $\mathcal{T}_{\mathcal{G}}$, and $(\boldsymbol{W}, \boldsymbol{w})$ its coset representative. In this way, the symmetry operations of $\mathcal{G}$ can be distributed into a finite set of infinite cosets, the elements of which are obtained by the combination of a coset representative $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ and the infinite set $\mathcal{T}_{\mathcal{G}} = \{(\boldsymbol{I}, \boldsymbol{t})\}$ of translations (*cf.* Section 1.3.3.2):

$$\mathcal{G} = \mathcal{T}_{\mathcal{G}} \cup \mathcal{T}_{\mathcal{G}}(\boldsymbol{W}_2, \boldsymbol{w}_2) \cup \cdots \cup \mathcal{T}_{\mathcal{G}}(\boldsymbol{W}_m, \boldsymbol{w}_m) \cup \cdots \cup \mathcal{T}_{\mathcal{G}}(\boldsymbol{W}_i, \boldsymbol{w}_i), \quad (1.4.2.1)$$

where $(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{I}, \boldsymbol{o})$ is omitted. Obviously, the coset representatives $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ of the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ represent in a clear and compact way the infinite number of symmetry operations of the space group $\mathcal{G}$. Each coset in the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ is characterized by its linear part $\boldsymbol{W}_j$ and its entries differ only by lattice translations. The translations $(\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}_{\mathcal{G}}$ form the first coset with the identity $(\boldsymbol{I}, \boldsymbol{o})$ as a coset representative. The symmetry operations with rotation part $\boldsymbol{W}_2$ form the second coset *etc*. The number of cosets equals the number of different matrices $\boldsymbol{W}_j$ of the symmetry operations of the space group. This number $[i]$ is always finite and is equal to the order of the point group $\mathcal{P}_{\mathcal{G}}$ of the space group (*cf.* Section 1.3.3.2).

For each space group, a set of coset representatives $\{(\boldsymbol{W}_j, \boldsymbol{w}_j), 1 \le j \le [i]\}$ of the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ is listed under the general-position block of the space-group tables. In general, any element of a coset may be chosen as a coset representative. For convenience, the representatives listed in the space-group tables are always chosen such that the components $w_{j,k}$, $k = 1, 2, 3$, of the translation parts $\boldsymbol{w}_j$ fulfil $0 \le w_{j,k} < 1$ (by subtracting integers). To save space, each matrix–column pair $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ is represented by the corresponding *coordinate triplet* (*cf.* Section 1.2.2.3 for the shorthand notation of matrix–column pairs).

Example

The right coset decomposition of $P2_1/c$, No. 14 (unique axis b, cell choice 1) with respect to its translation subgroup is shown in Table 1.4.2.6. All possible symmetry operations of $P2_1/c$ are distributed into four cosets:

The first column represents the infinitely many translations $t = (\boldsymbol{I}, \boldsymbol{t}) = x+u_1, y+u_2, z+u_3 = \{1|u_1, u_2, u_3\}$ of the translation subgroup $\mathcal{T}$ of $P2_1/c$. The numbers u_1, u_2 and u_3 are positive or negative integers. The identity operation $(\boldsymbol{I}, \boldsymbol{o})$ is usually chosen as a coset representative.

The third coset of the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ represents the infinite set of inversions $(-\boldsymbol{I}, \boldsymbol{t}) = \bar{x}+u_1, \bar{y}+u_2, \bar{z}+u_3 = \{\bar{1}|u_1, u_2, u_3\}$ of the space group $P2_1/c$ with inversion centres located at $u_1/2, u_2/2, u_3/2$ (*cf.* Section 1.2.2.4 for the determination of the location of the inversion centres). The inversion in the origin, *i.e.* $\bar{x}, \bar{y}, \bar{z} = \{\bar{1}|0\}$, is taken as a coset representative.

The coset representative of the second coset is the twofold screw rotation $\{2_{010}|0, \frac{1}{2}, \frac{1}{2}\}$ around the line $0, y, \frac{1}{4}$, followed by its infinite combinations with all lattice translations: $\bar{x}+u_1, y+\frac{1}{2}+u_2, \bar{z}+\frac{1}{2}+u_3 = \{2_{010}|u_1, \frac{1}{2}+u_2, \frac{1}{2}+u_3\}$. These are twofold screw rotations around the lines $u_1/2, y, u_3/2+\frac{1}{4}$ with screw components $\begin{pmatrix} 0 \\ \frac{1}{2}+u_2 \\ 0 \end{pmatrix}$.

The symmetry operations of the fourth column represented by $x+u_1, \bar{y}+\frac{1}{2}+u_2, z+\frac{1}{2}+u_3 = \{m_{010}|u_1, \frac{1}{2}+u_2, \frac{1}{2}+u_3\}$ correspond to glide reflections with glide components $\begin{pmatrix} u_1 \\ 0 \\ \frac{1}{2}+u_3 \end{pmatrix}$ through the (infinite) set of glide planes at $x, \frac{1}{4}, z$;

$x, \frac{3}{4}, z$; $x, \frac{5}{4}, z$; ...; $x, (2u_2+1)/4, z$. As usual, the symmetry operation with $u_1 = u_2 = u_3 = 0$, *i.e.* $x, \ \bar{y}+\frac{1}{2}, \ z+\frac{1}{2} = \{m_{010}|0, \frac{1}{2}, \frac{1}{2}\}$, is taken as a coset representative of the coset of glide reflections.

The coordinate triplets of the general-position block of $P2_1/c$ (unique axis b, cell choice 1) (*cf.* Fig. 1.4.2.1) correspond to the coset representatives of the decomposition of the group listed in the first line of Table 1.4.2.6.

When the space group is referred to a primitive basis (which is always done for '*P*' space groups), each coordinate triplet of the general-position block corresponds to one coset of $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$, *i.e.* the *multiplicity* of the general position and the number of cosets is the same. If, however, the space group is referred to a centred cell, then the complete set of general-position coordinate triplets is obtained by the combinations of the listed coordinate triplets with the centring translations. In this way, the total number of coordinate triplets per conventional unit cell, *i.e.* the multiplicity of the general position, is given by the product $[i] \times [p]$, where $[i]$ is the index of $\mathcal{T}_{\mathcal{G}}$ in $\mathcal{G}$ and $[p]$ is the index of the group of integer translations in the group $\mathcal{T}_{\mathcal{G}}$ of all (integer and centring) translations.

Example

The listing of the general position for the space–group type $Fmm2$ (42) of the space-group tables is reproduced in Fig. 1.4.2.2. The four entries, numbered (1) to (4), are to be taken as they are printed [indicated by (0, 0, 0)+]. The additional 12 more entries are obtained by adding the centring translations $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$ to the translation parts of the printed entries [indicated by $(0, \frac{1}{2}, \frac{1}{2})+$, $(\frac{1}{2}, 0, \frac{1}{2})+$ and $(\frac{1}{2}, \frac{1}{2}, 0)+$, respectively]. Altogether there are 16 entries, which is announced by the multiplicity of the general position, *i.e.* by the first number in the row. (The additional information specified on the left of the general-position block, namely the Wyckoff letter and the site symmetry, will be dealt with in Section 1.4.4.)

1.4.2.4. Additional symmetry operations and symmetry elements

The symmetry operations of a space group are conveniently partitioned into the cosets with respect to the translation subgroup. All operations which belong to the same coset have the same linear part and, if a single operation from a coset is given, all other operations in this coset are obtained by composition with a translation. However, not all symmetry operations in a coset with respect to the translation subgroup are operations of the same type and, furthermore, they may belong to element sets of different symmetry elements. In general, one can distinguish the following cases:

(i) The composition $W' = tW$ of a symmetry operation W with a translation t is an operation of the same type as W, with the same or a different type of symmetry element.

(ii) The composition $W' = tW$ is an operation of a different type to W with the same or a different type of symmetry element.

In order to distinguish the different cases, a closer analysis of the type of a symmetry operation and its symmetry element is required. These types, however, might be obscured by two obstacles:

(1) The origin in the chosen coordinate system might not lie on the geometric element of the symmetry operation. For example, the symmetry operation represented by the coordinate triplet $\bar{x}+1, \bar{y}+1, \bar{z}$ (*cf.* Section 1.4.2.3) is in fact an inversion through the point 1/2, 1/2, 0 and thus of the same type as the inversion $\{\bar{1}|0\}$ through the origin.

(2) The screw or glide part might not be reduced to a vector within the unit cell. For example, the symmetry operation $\bar{x}, \bar{y}, z+1$, which is a twofold screw rotation 2 (0, 0, 1) 0, 0, z along the c axis, is the composition of the twofold rotation $\bar{x}, \bar{y}, z$ with the lattice translation $t(0, 0, 1)$ along the screw axis. Although the two operations $\bar{x}, \bar{y}, z$ and $\bar{x}, \bar{y}, z+1$ are of different types, they are coaxial equivalents and belong to the element set of the same symmetry element (*cf.* Section 1.2.3).

These issues can be overcome by decomposing the translation part $\boldsymbol{w}$ of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ into an intrinsic translation part $\boldsymbol{w}_g$ which is fixed by the linear part $\boldsymbol{W}$ of W and thus parallel to the geometric element of W, and a location part $\boldsymbol{w}_l$, which is perpendicular to the intrinsic translation part. Note that the subspace of vectors fixed by $\boldsymbol{W}$ and the subspace perpendicular to this space of fixed vectors are complementary subspaces, *i.e.* their dimensions add up to 3, therefore this decomposition is always possible.

The procedure for determining the intrinsic translation part of a symmetry operation is described in Section 1.2.2.4, and is based on the fact that the kth power of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ with linear part $\boldsymbol{W}$ of order k must be a pure translation, *i.e.* $W^k = (\boldsymbol{I}, \boldsymbol{t})$ for some lattice translation $\boldsymbol{t}$. The *intrinsic translation part* of W is then defined as $\boldsymbol{w}_g = \frac{1}{k}\boldsymbol{t}$.

The difference $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{w}_g$ is perpendicular to $\boldsymbol{w}_g$ and it is called the *location part* of $\boldsymbol{w}$. This terminology is justified by the fact that the location part can be reduced to $\boldsymbol{o}$ by an origin shift, *i.e.* the location part indicates whether the origin of the chosen coordinate system lies on the geometric element of W.

The transformation of point coordinates and matrix–column pairs under an origin shift is explained in detail in Sections 1.5.1.3 and 1.5.2.3, and the complete procedure for determining the additional symmetry operations will be discussed in the context of the synoptic tables in Section 1.5.4. In this section we will restrict ourselves to a detailed discussion of two examples which illustrate typical phenomena.

Example 1

Consider a space group of type $Fmm2$ (42). The information on the general position and on the symmetry operations given in the space-group tables are reproduced in Fig. 1.4.2.2. From this information one deduces that coset representatives with respect to the translation subgroup are the identity element $W_1 = x, y, z$, a rotation $W_2 = \bar{x}, \bar{y}, z$ with the c axis as geometric element, a reflection $W_3 = x, \bar{y}, z$ with the plane $x, 0, z$ as geometric element and a reflection $W_4 = \bar{x}, y, z$ with the plane $0, y, z$ as geometric element (with the indices following the numbering in the table).

Composing these coset representatives with the centring translations $t(0, \frac{1}{2}, \frac{1}{2})$, $t(\frac{1}{2}, 0, \frac{1}{2})$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ gives rise to elements in the same cosets, but with different types of symmetry operations and symmetry elements in several cases.

(i) $(0, \frac{1}{2}, \frac{1}{2})$: The composition of the rotation W_2 with $t(0, \frac{1}{2}, \frac{1}{2})$ results in the symmetry operation $\bar{x}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$, which is a twofold screw rotation with screw axis $0, \frac{1}{4}, z$. This means that both the type of the symmetry operation and the location of the geometric element are changed. Composing the reflection W_3 with $t(0, \frac{1}{2}, \frac{1}{2})$ gives the symmetry operation $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$, which is a c glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the b axis relative to the geometric element of W_3. In the composition of W_4 with $t(0, \frac{1}{2}, \frac{1}{2})$, the translation lies

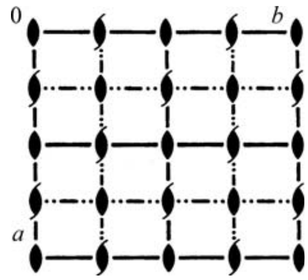

Figure 1.4.2.3
Symmetry-element diagram for space group *Fmm*2 (42) (orthogonal projection along [001]).

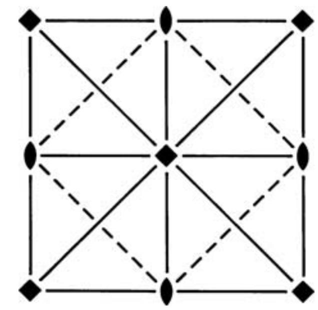

Figure 1.4.2.5
Symmetry-element diagram for space group *P*4*mm* (99) (orthogonal projection along [001]).

in the plane forming the geometric element of W_4. The geometric element of the resulting symmetry operation $\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$ is still the plane $0, y, z$, but the symmetry operation is now an *n* glide, *i.e.* a glide reflection with diagonal glide vector.

(ii) $(\frac{1}{2}, 0, \frac{1}{2})$: Analogous to the first centring translation, the composition of W_2 with $t(\frac{1}{2}, 0, \frac{1}{2})$ results in a twofold screw rotation with screw axis $\frac{1}{4}, 0, z$ as geometric element. The roles of the reflections W_3 and W_4 are interchanged, because the translation vector now lies in the plane forming the geometric element of W_3. Therefore, the composition of W_3 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an *n* glide with the plane $x, 0, z$ as geometric element, whereas the composition of W_4 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is a *c* glide with the plane $\frac{1}{4}, y, z$ as geometric element.

(iii) $(\frac{1}{2}, \frac{1}{2}, 0)$: Because this translation vector lies in the plane perpendicular to the rotation axis of W_2, the composition of W_2 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is still a twofold rotation, *i.e.* a symmetry operation of the same type, but the rotation axis is shifted by $\frac{1}{4}, \frac{1}{4}, 0$ in the *xy* plane to become the axis $\frac{1}{4}, \frac{1}{4}, z$. The composition of W_3 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ results in the symmetry operation $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$, which is an *a* glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the *b* axis relative to the geometric element of W_3. Similarly, the composition of W_4 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is a *b* glide with the plane $\frac{1}{4}, y, z$ as geometric element.

In this example, all additional symmetry operations are listed in the symmetry-operations block of the space-group tables of *Fmm*2 because they are due to compositions of the coset representatives with centring translations.

The additional symmetry operations can easily be recognized in the symmetry-element diagrams (*cf.* Section 1.4.2.5). Fig. 1.4.2.3 shows the symmetry-element diagram of *Fmm*2 for the projection along the *c* axis. One sees that twofold rotation axes alternate with twofold screw axes and that mirror planes alternate with 'double' or *e*-glide planes, *i.e.* glide planes with two glide vectors. For example, the dot–dashed lines at $x=\frac{1}{4}$ and $x=\frac{3}{4}$ in Fig. 1.4.2.3 represent the *b* and *c* glides with normal vector along the *a* axis [for a discussion of *e*-glide notation, see Sections 1.2.3 and 2.1.2, and de Wolff *et al.*, 1992].

Example 2

In a space group of type *P*4*mm* (99), representatives of the space group with respect to the translation subgroup are the powers of a fourfold rotation and reflections with normal vectors along the *a* and the *b* axis and along the diagonals [110] and [1$\bar{1}$0] (*cf.* Fig. 1.4.2.4).

In this case, additional symmetry operations occur although there are no centring translations. Consider for example the reflection W_8 with the plane x, x, z as geometric element. Composing this reflection with the translation $t(1,0,0)$ gives rise to the symmetry operation represented by $y+1, x, z$. This operation maps a point with coordinates $x+\frac{1}{2}, x, z$ to $x+1, x+\frac{1}{2}, z$ and is thus a glide reflection with the plane $x+\frac{1}{2}, x, z$ as geometric element and $(\frac{1}{2}, \frac{1}{2}, 0)$ as glide vector. In a similar way, composing the other diagonal reflection with translations yields further glide reflections.

These glide reflections are symmetry operations which are not listed in the symmetry-operations block, although they are clearly of a different type to the operations given there. However, in the symmetry-element diagram as shown in Fig. 1.4.2.5, the corresponding symmetry elements are displayed as diagonal dashed lines which alternate with the solid diagonal lines representing the diagonal reflections.

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*g*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^{+} $0,0,z$	(4) 4^{-} $0,0,z$
(5) *m* $x,0,z$	(6) *m* $0,y,z$	(7) *m* $x,\bar{x},z$	(8) *m* x,x,z

Figure 1.4.2.4
General-position and symmetry-operations blocks as given in the space-group tables for space group *P*4*mm* (99).

1.4.2.5. Space-group diagrams

In the space-group tables of Chapter 2.3, for each space group there are at least two diagrams displaying the symmetry (there are more diagrams for space groups of low symmetry). The *symmetry-element* diagram displays the location and orientation of the symmetry elements of the space group. The *general-position* diagrams show the arrangement of a set of symmetry-equivalent points of the general position. Because of the periodicity of the arrangements, the presentation of the contents of one unit cell is sufficient. Both types of diagrams are orthogonal projections of the space-group unit cell onto the plane of projection along a basis vector of the conventional crystallographic coordinate system. The symmetry elements of triclinic, monoclinic and orthorhombic groups are shown in three different projections along the basis vectors.

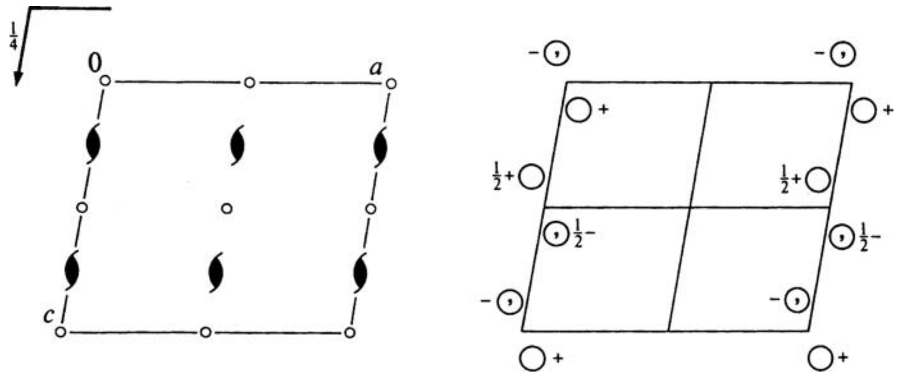

Figure 1.4.2.6
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2_1/c$, No. 14 (unique axis b, cell choice 1).

The thin lines outlining the projection are the traces of the side planes of the unit cell.

Detailed explanations of the diagrams of space groups are found in Section 2.1.3.6. In this section, after a very brief introduction to the diagrams, we will focus mainly on certain important but very often overlooked features of the diagrams.

Symmetry-element diagram

The graphical symbols of the symmetry elements used in the diagrams are explained in Section 2.1.2. The heights along the projection direction above the plane of the diagram are indicated for rotation or screw axes and mirror or glide planes parallel to the projection plane, for rotoinversion axes and inversion centres. The heights (if different from zero) are given as fractions of the shortest translation vector along the projection direction. In Fig. 1.4.2.6 (left) the symmetry elements of $P2_1/c$ (unique axis b, cell choice 1) are represented graphically in a projection of the unit cell along the monoclinic axis **b**. The directions of the basis vectors **c** and **a** can be read directly from the figure. The origin (upper left corner of the unit cell) lies on a centre of inversion indicated by a small open circle. The black lenticular symbols with tails represent the twofold screw axes parallel to **b**. The c-glide plane at height $\frac{1}{4}$ along **b** is shown as a bent arrow with the arrowhead pointing along **c**.

The crystallographic symmetry operations are visualized geometrically by the related symmetry elements. Whereas the symmetry element of a symmetry operation is uniquely defined, more than one symmetry operation may belong to the same symmetry element (*cf.* Section 1.2.3). The following examples illustrate some important features of the diagrams related to the fact that the symmetry-element symbols that are displayed visualize all symmetry operations that belong to the element sets of the symmetry elements.

Examples

(1) *Visualization of the twofold screw rotations of $P2_1/c$* (Fig. 1.4.2.6). The second coset of the decomposition of $P2_1/c$ with respect to its translation subgroup shown in Table 1.4.2.6 is formed by the infinite set of twofold screw rotations represented by the coordinate triplets $\bar{x}+u_1$, $y+\frac{1}{2}+u_2, \bar{z}+\frac{1}{2}+u_3$ (where u_1, u_2, u_3 are integers). To analyse how these symmetry operations are visualized, it is convenient to consider two special cases:

(i) $u_2 = 0$, *i.e.* $\bar{x}+u_1,\ y+\frac{1}{2},\ \bar{z}+\frac{1}{2}+u_3$ = $\{2_{010}|u_1, \frac{1}{2}, \frac{1}{2}+u_3\}$; these operations correspond to twofold screw rotations around the infinitely many screw axes parallel to the line $0, y, \frac{1}{4}$, *i.e.* around the lines $u_1/2, y, u_3/2+\frac{1}{4}$. The symbols of the symmetry elements (*i.e.* of the twofold screw axes) located in the unit cell at $0, y, \frac{1}{4}$; $0, y, \frac{3}{4}$; $\frac{1}{2}, y, \frac{1}{4}$; $\frac{1}{2}, y, \frac{3}{4}$ (and the translationally equivalent $1, y, \frac{1}{4}$ and $1, y, \frac{3}{4}$) are shown in the symmetry-element diagram (Fig. 1.4.2.6);

(ii) $u_1 = u_3 = 0$, *i.e.* $\bar{x},\ y+\frac{1}{2}+u_2,\ \bar{z}+\frac{1}{2}$ = $\{2_{010}|0, \frac{1}{2}+u_2, \frac{1}{2}\}$; these symmetry operations correspond to screw rotations around the line $0, y, \frac{1}{4}$ with screw components $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots$, *i.e.* with a screw component $\frac{1}{2}$ to which all lattice translations parallel to the screw axis are added. These operations, infinite in number, share the same geometric element, *i.e.* they form the element set of the same symmetry element, and geometrically they are represented just by one graphical symbol on the symmetry-element diagrams located exactly at $0, y, \frac{1}{4}$.

(iii) The rest of the symmetry operations in the coset, *i.e.* those with the translation parts $\begin{pmatrix} u_1 \\ \frac{1}{2}+u_2 \\ \frac{1}{2}+u_3 \end{pmatrix}$, are combinations of the two special cases above.

(2) *Inversion centres of $P2_1/c$* (Fig. 1.4.2.6). The element set of an inversion centre consists of only one symmetry operation, *viz.* the inversion through the point located at the centre. In other words, to each inversion centre displayed on a symmetry-element diagram there corresponds one symmetry operation of inversion. The infinitely many inversions $(-\boldsymbol{I}, \boldsymbol{t})$ = $\bar{x}+u_1, \bar{y}+u_2, \bar{z}+u_3$ = $\{\bar{1}|u_1, u_2, u_3\}$ of $P2_1/c$ are located at points $u_1/2$, $u_2/2, u_3/2$. Apart from translational equivalence, there are eight centres located in the unit cell: four at $y = 0$, namely at $0, 0, 0$; $\frac{1}{2}, 0, 0$; $0, 0, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{2}$ and four at height $\frac{1}{2}$ of b. It is important to note that only inversion centres at $y = 0$ are indicated on the diagram.

A similar rule is applied to all pairs of symmetry elements of the same type (such as *e.g.* twofold rotation axes, planes *etc.*) whose heights differ by $\frac{1}{2}$ of the shortest lattice direction along the projection direction. For example, the c-glide plane symbol in Fig. 1.4.2.6 with the fraction $\frac{1}{4}$ next to it represents not only the c-glide plane located at height $\frac{1}{4}$ but also the one at height $\frac{3}{4}$.

(3) *Glide reflections visualized by mirror planes*. As discussed in Section 1.2.3, the element set of a mirror or glide plane consists of a defining operation and all its coplanar equivalents (*cf.* Table 1.2.3.1). The corresponding symmetry element is a mirror plane if among the infinite set of the coplanar glide reflections there is one with zero glide vector. Thus, the symmetry element is a mirror plane and

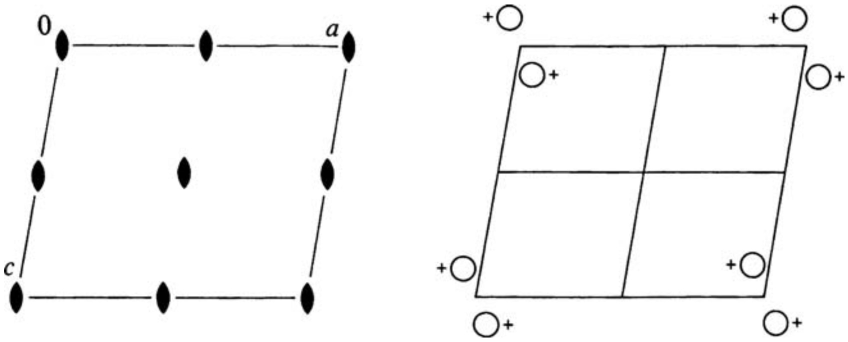

Figure 1.4.2.7
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2$, No. 3 (unique axis b, cell choice 1).

the graphical symbol for a mirror plane is used for its representation on the symmetry-element diagrams of the space groups. For example, the mirror plane $0, y, z$ shown on the symmetry-element diagram of $Fmm2$ (42), *cf.* Fig. 1.4.2.3, represents all glide reflections of the element set of the defining operation $0, y, z$ [symmetry operation (4) of the general-position $(0, 0, 0)+$ set, *cf.* Fig. 1.4.2.2], including the n-glide reflection $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ [entry (4) of the general-position $(0, \frac{1}{2}, \frac{1}{2})+$ set]. In a similar way, the graphical symbols of the mirror planes $x, 0, z$ also represent the n-glide reflections $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ [entry (3) of the general-position $(\frac{1}{2}, 0, \frac{1}{2})+$ set] of $Fmm2$.

General-position diagram

The graphical presentations of the space-group symmetries provided by the general-position diagrams consist of a set of general-position points which are symmetry equivalent under the symmetry operations of the space group. Starting with a point in the upper left corner of the unit cell, indicated by an open circle with a sign '+', all the displayed points inside and near the unit cell are images of the starting point under some symmetry operation of the space group. Because of the one-to-one correspondence between the image points and the symmetry operations, the number of general-position points in the unit cell (excluding the points that are equivalent by integer translations) equals the multiplicity of the general position. The coordinates of the points in the projection plane can be read directly from the diagram. For all systems except cubic, only one parameter is necessary to describe the height along the projection direction. For example, if the height of the starting point above the projection plane is indicated by a '+' sign, then signs '+', '−' or their combinations with fractions (*e.g.* $\frac{1}{2}+$, $\frac{1}{2}-$ *etc.*) are used to specify the heights of the image points. A circle divided by a vertical line represents two points with different coordinates along the projection direction but identical coordinates in the projection plane. A comma ',' in the circle indicates an image point obtained by a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ of the second kind [*i.e.* with $\det(\boldsymbol{W}) = -1$, *cf.* Section 1.2.2].

Example

The general-position diagram of $P2_1/c$ (unique axis b, cell choice 1) is shown in Fig. 1.4.2.6 (right). The open circles indicate the location of the four symmetry-equivalent points of the space group within the unit cell along with additional eight translation-equivalent points to complete the presentation. The circles with a comma inside indicate the image points generated by operations of the second kind – inversions and glide planes in the present case. The fractions and signs close to the circles indicate their heights in units of b of the symmetry-equivalent points along the monoclinic axis. For example, $\frac{1}{2}-$ is a shorthand notation for $\frac{1}{2} - y$.

Notes:

(1) The close relation between the symmetry-element and the general-position diagrams is obvious. For example, the points shown on the general-position diagram are images of a general-position point under the action of the space-group symmetry operations displayed by the corresponding symmetry elements on the symmetry-element diagram. With

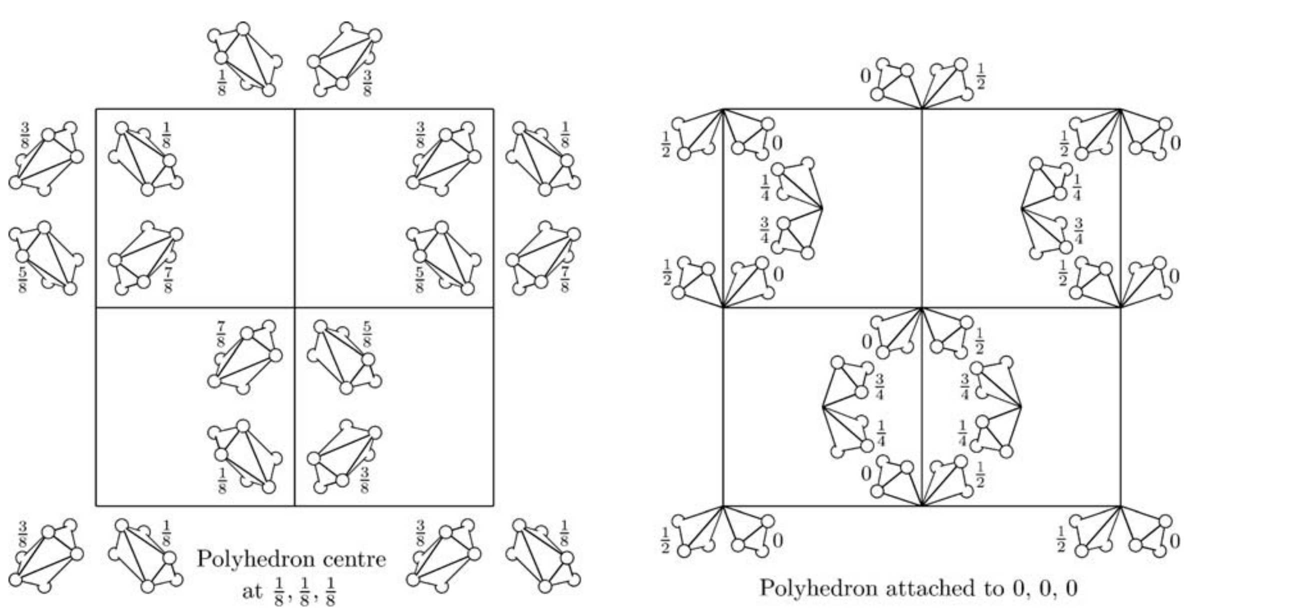

Figure 1.4.2.8
General-position diagrams for the space group $I4_132$ (214). Left: polyhedra (twisted trigonal antiprisms) with centres at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points (site-symmetry group .32). Right: polyhedra (sphenoids) attached to 0, 0, 0 and its equivalent points (site-symmetry group .3.).

some practice each of the diagrams can be generated from the other. In a number of texts, the two diagrams are considered as completely equivalent descriptions of the same space group. This statement is true for most of the space groups. However, there are a number of space groups for which the point configuration displayed on the general-position diagram has higher symmetry than the generating space group (Suescun & Nespolo, 2012; Müller, 2012). For example, consider the diagrams of the space group $P2$, No. 3 (unique axis b, cell choice 1) shown in Fig. 1.4.2.7. It is easy to recognise that, apart from the twofold rotations, the point configuration shown in the general-position diagram is symmetric with respect to a reflection through a plane containing the general-position points, and as a result the space group of the general-position configuration is of $P2/m$ type, and not of $P2$. There are a number of space groups for which the general-position diagram displays higher space-group symmetry, for example: $P1$, $P2_1$, $P4mm$, $P6$ *etc.* The analysis of the eigensymmetry groups of the general-position orbits results in a systematic procedure for the determination of such space groups: the general-position diagrams do not reflect the space-group symmetry correctly if the general-position orbits are *non-characteristic*, *i.e.* their eigensymmetry groups are supergroups of the space groups. (An introduction to terms like eigensymmetry groups, characteristic and non-characteristic orbits, and further discussion of space groups with non-characteristic general-position orbits are given in Section 1.4.4.4.)

(2) The graphical presentation of the general-position points of cubic groups is more difficult: three different parameters are required to specify the height of the points along the projection direction. To make the presentation clearer, the general-position points are grouped around points of higher site symmetry and represented in the form of polyhedra. For most of the space groups the initial general point is taken as 0.048, 0.12, 0.089, and the polyhedra are centred at 0, 0, 0 (and its equivalent points). Additional general-position diagrams are shown for space groups with special sites different from 0, 0, 0 that have site-symmetry groups of equal or higher order. Consider, for example, the two general-position diagrams of the space group $I4_132$ (214) shown in Fig. 1.4.2.8. The polyhedra of the left-hand diagram are centred at special points of highest site-symmetry, namely, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points in the unit cell. The site-symmetry groups are of the type 32 leading to polyhedra in the form of *twisted trigonal antiprisms* (*cf.* Table 3.2.3.2). The polyhedra (sphenoids) of the right-hand diagram are attached to the origin 0, 0, 0 and its equivalent points in the unit cell, site-symmetry group of the type 3. The fractions attached to the polyhedra indicate the heights of the high-symmetry points along the projection direction (*cf.* Section 2.1.3.6 for further explanations of the diagrams).

Table 1.4.3.1
Sequence of generators for the crystal classes

The space-group generators differ from those listed here by their glide or screw components. The generator 1 is omitted, except for crystal class 1. The generators are represented by the corresponding Seitz symbols (*cf.* Tables 1.4.2.1–1.4.2.3). Following the conventions, the subscript of a symbol denotes the characteristic direction of that operation, where necessary. For example, the subscripts 001, 010, 110 *etc.* refer to the directions [001], [010], [110] *etc.* For mirror reflections m, the 'direction of m' refers to the normal of the mirror plane.

Hermann–Mauguin symbol of crystal class	Generators g_i (sequence left to right)
1	1
$\bar{1}$	$\bar{1}$
2	2
m	m
$2/m$	$2, \bar{1}$
222	$2_{001}, 2_{010}$
$mm2$	$2_{001}, m_{010}$
mmm	$2_{001}, 2_{010}, \bar{1}$
4	$2_{001}, 4^+_{001}$
$\bar{4}$	$2_{001}, \bar{4}^+_{001}$
$4/m$	$2_{001}, 4^+_{001}, \bar{1}$
422	$2_{001}, 4^+_{001}, 2_{010}$
$4mm$	$2_{001}, 4^+_{001}, m_{010}$
$\bar{4}2m$	$2_{001}, \bar{4}^+_{001}, 2_{010}$
$\bar{4}m2$	$2_{001}, \bar{4}^+_{001}, m_{010}$
$4/mmm$	$2_{001}, 4^+_{001}, 2_{010}, \bar{1}$
3	3^+_{001}
(rhombohedral coordinates	3^+_{111})
$\bar{3}$	$3^+_{001}, \bar{1}$
(rhombohedral coordinates	$3^+_{111}, \bar{1}$
321	$3^+_{001}, 2_{110}$
(rhombohedral coordinates	$3^+_{111}, 2_{\bar{1}01}$)
312	$3^+_{001}, 2_{1\bar{1}0}$
$3m1$	$3^+_{001}, m_{110}$
(rhombohedral coordinates	$3^+_{111}, m_{\bar{1}01}$)
$31m$	$3^+_{001}, m_{1\bar{1}0}$
$\bar{3}m1$	$3^+_{001}, 2_{110}, \bar{1}$
(rhombohedral coordinates	$3^+_{111}, 2_{\bar{1}01}, \bar{1}$)
$\bar{3}1m$	$3^+_{001}, 2_{1\bar{1}0}, \bar{1}$
6	$3^+_{001}, 2_{001}$
$\bar{6}$	$3^+_{001}, m_{001}$
$6/m$	$3^+_{001}, 2_{001}, \bar{1}$
622	$3^+_{001}, 2_{001}, 2_{110}$
$6mm$	$3^+_{001}, 2_{001}, m_{110}$
$\bar{6}m2$	$3^+_{001}, m_{001}, m_{110}$
$\bar{6}2m$	$3^+_{001}, m_{001}, 2_{110}$
$6/mmm$	$3^+_{001}, 2_{001}, 2_{110}, \bar{1}$
23	$2_{001}, 2_{010}, 3^+_{111}$
$m\bar{3}$	$2_{001}, 2_{010}, 3^+_{111}, \bar{1}$
432	$2_{001}, 2_{010}, 3^+_{111}, 2_{110}$
$\bar{4}3m$	$2_{001}, 2_{010}, 3^+_{111}, m_{1\bar{1}0}$
$m\bar{3}m$	$2_{001}, 2_{010}, 3^+_{111}, 2_{110}, \bar{1}$

1.4.3. Generation of space groups

By H. Wondratschek

In group theory, a *set of generators* of a group is a set of group elements such that each group element may be obtained as a finite ordered product of the generators. For space groups of one, two and three dimensions, generators may always be chosen and ordered in such a way that each symmetry operation W can be written as the product of powers of h generators g_j ($j = 1, 2, \ldots, h$). Thus,

$$W = g_h^{k_h} \cdot g_{h-1}^{k_{h-1}} \cdot \ldots \cdot g_p^{k_p} \cdot \ldots \cdot g_3^{k_3} \cdot g_2^{k_2} \cdot g_1,$$

where the powers k_j are positive or negative integers (including zero). The description of a group by means of generators has the advantage of compactness. For instance, the 48 symmetry operations in point group $m\bar{3}m$ can be described by two

Table 1.4.3.2
Generation of the space group $P6_122 \equiv D_6^2$ (178)

The entries in the second column designated by the numbers (1)–(12) correspond to the coordinate triplets of the general position of $P6_122$.

	Coordinate triplets	Symmetry operations
g_1	(1) x, y, z;	Identity I
g_2	$t(100)$	Generating translations
g_3	$t(010)$	
g_4	$t(001)$	
	The group $\mathcal{G}_4 \equiv \mathcal{T}$ of all translations of $P6_122$ has been generated	
g_5	(2) $\bar{y}, x-y, z+\frac{1}{3}$;	Threefold screw rotation
g_5^2	(3) $\bar{x}+y, \bar{x}, z+\frac{2}{3}$;	Threefold screw rotation
$g_5^3 = t(001)$:	Now the space group $\mathcal{G}_5 \equiv P3_1$ has been generated	
g_6	(4) $\bar{x}, \bar{y}, z+\frac{1}{2}$;	Twofold screw rotation
$g_6 * g_5$	(5) $y, \bar{x}+y, z+\frac{5}{6}$;	Sixfold screw rotation
$g_6 * g_5^2$	$x-y, x, z+\frac{7}{6} \sim$ (6) $x-y, x, z+\frac{1}{6}$;	Sixfold screw rotation
$g_6^2 = t(001)$:	Now the space group $\mathcal{G}_6 \equiv P6_1$ has been generated	
g_7	(7) $y, x, \bar{z}+\frac{1}{3}$;	Twofold rotation, direction of axis [110]
$g_7 * g_5$	(8) $x-y, \bar{y}, \bar{z}$;	Twofold rotation, axis [100]
$g_7 * g_5^2$	$\bar{x}, \bar{x}+y, \bar{z}-\frac{1}{3} \sim$ (9) $\bar{x}, \bar{x}+y, \bar{z}+\frac{2}{3}$;	Twofold rotation, axis [010]
$g_7 * g_6$	$\bar{y}, \bar{x}, \bar{z}-\frac{1}{6} \sim$ (10) $\bar{y}, \bar{x}, \bar{z}+\frac{5}{6}$;	Twofold rotation, axis $[1\bar{1}0]$
$g_7 * g_6 * g_5$	$\bar{x}+y, y, \bar{z}-\frac{1}{2} \sim$ (11) $\bar{x}+y, y, \bar{z}+\frac{1}{2}$;	Twofold rotation, axis [120]
$g_7 * g_6 * g_5^2$	$x, x-y, \bar{z}-\frac{5}{6} \sim$ (12) $x, x-y, \bar{z}+\frac{1}{6}$;	Twofold rotation, axis [210]
$g_7^2 = I$	$\mathcal{G}_7 \sim P6_122$	

generators. Different choices of generators are possible. For the space-group tables, generators and generating procedures have been chosen such as to make the entries in the blocks 'General position' (*cf.* Section 2.1.3.11) and 'Symmetry operations' (*cf.* Section 2.1.3.9) as transparent as possible. Space groups of the same crystal class are generated in the same way (see Table 1.4.3.1 for the sequences that have been chosen), and the aim has been to accentuate important subgroups of space groups as much as possible. Accordingly, a process of generation in the form of a *composition series* has been adopted, see Ledermann (1976). The generator g_1 is defined as the identity operation, represented by (1) x, y, z. The generators g_2, g_3, and g_4 are the translations with translation vectors **a**, **b** and **c**, respectively. Thus, the coefficients k_2, k_3 and k_4 may have any integral value. If centring translations exist, they are generated by translations g_5 (and g_6 in the case of an F lattice) with translation vectors **d** (and **e**). For a C lattice, for example, **d** is given by $\mathbf{d} = \frac{1}{2}(\mathbf{a}+\mathbf{b})$. The exponents k_5 (and k_6) are restricted to the following values:

Lattice letter A, B, C, I: $k_5 = 0$ or 1.
Lattice letter R (hexagonal axes): $k_5 = 0$, 1 or 2.
Lattice letter F: $k_5 = 0$ or 1; $k_6 = 0$ or 1.

As a consequence, any translation t of $\mathcal{G}$ with translation vector

$$\mathbf{t} = k_2\mathbf{a} + k_3\mathbf{b} + k_4\mathbf{c}\,(+k_5\mathbf{d} + k_6\mathbf{e})$$

can be obtained as a product

$$t = (g_6)^{k_6}.(g_5)^{k_5}.g_4^{k_4}.g_3^{k_3}.g_2^{k_2}.g_1,$$

where $k_2, \ldots, k_6$ are integers determined by t. The generators g_6 and g_5 are enclosed between parentheses because they are effective only in centred lattices.

The remaining generators generate those symmetry operations that are not translations. They are chosen in such a way that only terms g_j or g_j^2 occur. For further specific rules, see below.

The process of generating the entries of the space-group tables may be demonstrated by the example in Table 1.4.3.2, where $\mathcal{G}_j$ denotes the group generated by $g_1, g_2, \ldots, g_j$. For $j \geq 5$, the next generator g_{j+1} is introduced when $g_j^{k_j} \in \mathcal{G}_{j-1}$, because in this case no new symmetry operation would be generated by $g_j^{k_j}$. The generating process is terminated when there is no further generator. In the present example, g_7 completes the generation: $\mathcal{G}_7 \equiv P6_122$ (178).

1.4.3.1. Selected order for non-translational generators

For the non-translational generators, the following sequence has been adopted:

(*a*) In all centrosymmetric space groups, an inversion (if possible at the origin O) has been selected as the last generator.

(*b*) Rotations precede symmetry operations of the second kind. In crystal classes $\bar{4}2m$ and $\bar{4}m2$ and $\bar{6}2m$ and $\bar{6}m2$, as an exception, $\bar{4}$ and $\bar{6}$ are generated first in order to take into account the conventional choice of origin in the fixed points of $\bar{4}$ and $\bar{6}$.

(*c*) The non-translational generators of space groups with C, A, B, F, I or R symbols are those of the corresponding space group with a P symbol, if possible. For instance, the generators of $I2_12_12_1$ (24) are those of $P2_12_12_1$ (19) and the generators of *Ibca* (73) are those of *Pbca* (61), apart from the centring translations.

Exceptions: *I4cm* (108) and *I4*/*mcm* (140) are generated *via* *P4cc* (103) and *P4*/*mcc* (124), because *P4cm* and *P4*/*mcm* do not exist. In space groups with d glides (except $I\bar{4}2d$, No. 122) and also in $I4_1/a$ (88), the corresponding rotation subgroup has been generated first. The generators of this subgroup are the same as those of the corresponding space group with a lattice symbol P.

Example
$F4_1/d\bar{3}2/m$ (227):
$P4_132$ (213) $\longrightarrow$ $F4_132$ (210) $\longrightarrow$ $F4_1/d\bar{3}2/m$.

(*d*) In some cases, rule (*c*) could not be followed without breaking rule (*a*), *e.g.* in *Cmme* (67). In such cases, the generators are chosen to correspond to the Hermann–Mauguin symbol as far as possible. For instance, the generators (apart from centring) of *Cmme* and *Imma* (74) are those of *Pmmb*, which is a non-standard setting of *Pmma* (51). (A combination of the generators of *Pmma* with the *C*- or *I*-centring translation results in non-standard settings of *Cmme* and *Imma*.)

For the space groups with lattice symbol *P*, the generation procedure has given the same triplets (except for their sequence) as in *IT* (1952). In non-*P* space groups, the triplets listed sometimes differ from those of *IT* (1952) by a centring translation.

1.4.4. General and special Wyckoff positions

By B. Souvignier

One of the first tasks in the analysis of crystal patterns is to determine the actual positions of the atoms. Since the full crystal pattern can be reconstructed from a single unit cell or even an asymmetric unit, it is clearly sufficient to focus on the atoms inside such a restricted volume. What one observes is that the atoms typically do not occupy arbitrary positions in the unit cell, but that they often lie on geometric elements, *e.g.* reflection planes or lines along rotation axes. It is therefore very useful to analyse the symmetry properties of the points in a unit cell in order to predict likely positions of atoms.

We note that in this chapter all statements and definitions refer to the usual three-dimensional space $\mathbb{E}^3$, but also can be formulated, *mutatis mutandis*, for plane groups acting on $\mathbb{E}^2$ and for higher-dimensional groups acting on *n*-dimensional space $\mathbb{E}^n$.

1.4.4.1. Crystallographic orbits

Since the operations of a space group provide symmetries of a crystal pattern, two points X and Y that are mapped onto each other by a space-group operation are regarded as being *geometrically equivalent*. Starting from a point $X \in \mathbb{E}^3$, infinitely many points Y equivalent to X are obtained by applying all space-group operations $g = (\boldsymbol{W}, \boldsymbol{w})$ to X: $Y = g(X) = (\boldsymbol{W}, \boldsymbol{w})X = (\boldsymbol{W}X + \boldsymbol{w})$.

Definition

For a space group $\mathcal{G}$ acting on the three-dimensional space $\mathbb{E}^3$, the (infinite) set

$$\mathcal{O} = \mathcal{G}(X) := \{g(X) | g \in \mathcal{G}\}$$

is called the *orbit of X under* $\mathcal{G}$.

The orbit of X is the smallest subset of $\mathbb{E}^3$ that contains X and is closed under the action of $\mathcal{G}$. It is also called a *crystallographic orbit*.

Every point in direct space $\mathbb{E}^3$ belongs to precisely one orbit under $\mathcal{G}$ and thus the orbits of $\mathcal{G}$ partition the direct space into disjoint subsets. It is clear that an orbit is completely determined by its points in the unit cell, since translating the unit cell by the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ entirely covers $\mathbb{E}^3$.

It may happen that two different symmetry operations g and h in $\mathcal{G}$ map X to the same point. Since $g(X) = h(X)$ implies that $h^{-1}g(X) = X$, the point X is fixed by the nontrivial operation $h^{-1}g$ in $\mathcal{G}$.

Definition

The subgroup $\mathcal{S}_X = \mathcal{S}_{\mathcal{G}}(X) := \{g \in \mathcal{G} | g(X) = X\}$ of symmetry operations from $\mathcal{G}$ that fix X is called the *site-symmetry group of X in* $\mathcal{G}$.

Since translations, glide reflections and screw rotations fix no point in $\mathbb{E}^3$, a site-symmetry group $\mathcal{S}_X$ never contains operations of these types and thus consists only of reflections, rotations, inversions and rotoinversions. Because of the absence of translations, $\mathcal{S}_X$ contains at most one operation from a coset $\mathcal{T}g$ relative to the translation subgroup $\mathcal{T}$ of $\mathcal{G}$, since otherwise the quotient of two such operations tg and $t'g$ would be the nontrivial translation $tgg^{-1}t'^{-1} = tt'^{-1}$ (see Chapter 1.3 for a discussion of coset decompositions). In particular, the operations in $\mathcal{S}_X$ all have different linear parts and because these linear parts form a subgroup of the point group $\mathcal{P}$ of $\mathcal{G}$, the order of the site-symmetry group $\mathcal{S}_X$ is a divisor of the order of the point group of $\mathcal{G}$.

The site-symmetry group of a point X is thus a finite subgroup of the space group $\mathcal{G}$, a subgroup which is isomorphic to a subgroup of the point group $\mathcal{P}$ of $\mathcal{G}$.

Example

For a space group $\mathcal{G}$ of type $P\bar{1}$, the site-symmetry group of the origin $X = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ is clearly generated by the inversion in the origin: $\{\bar{1}|0\}(X) = X$. On the other hand, the point $Y = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$ is fixed by the inversion in Y, *i.e.*

$$\{\bar{1}|1, 0, 1\}(Y) = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix} = Y.$$

The symmetry operation $\{\bar{1}|1, 0, 1\}$ also belongs to $\mathcal{G}$ and generates the site-symmetry group of Y. The site-symmetry groups $\mathcal{S}_X = \{\{1|0\}, \{\bar{1}|0\}\}$ of X and $\mathcal{S}_Y = \{\{1|0\}, \{\bar{1}|1, 0, 1\}\}$ of Y are thus different subgroups of order 2 of $\mathcal{G}$ which are isomorphic to the point group of $\mathcal{G}$ (which is generated by $\bar{1}$).

The order $|\mathcal{S}_X|$ of the site-symmetry group $\mathcal{S}_X$ is closely related to the number of points in the orbit of X that lie in the unit cell. An application of the orbit–stabilizer theorem (see Section 1.1.7) yields the crucial observation that each point $Y = g(X)$ in the orbit of X under $\mathcal{G}$ is obtained precisely $|\mathcal{S}_X|$ times as an orbit point: for each $h \in \mathcal{S}_X$ one has $gh(X) = g(X) = Y$ and conversely $g'(X) = g(X)$ implies that $g^{-1}g' = h \in \mathcal{S}_X$ and thus $g' = gh$ for an operation h in $\mathcal{S}_X$.

Assuming first that we are dealing with a space group $\mathcal{G}$ described by a *primitive* lattice, each coset of $\mathcal{G}$ relative to the translation subgroup $\mathcal{T}$ contains precisely one operation g such that $g(X)$ lies in the primitive unit cell. Since the number of cosets equals the order $|\mathcal{P}|$ of the point group $\mathcal{P}$ of $\mathcal{G}$ and since each orbit point is obtained $|\mathcal{S}_X|$ times, it follows that the number of orbit points in the unit cell is $|\mathcal{P}|/|\mathcal{S}_X|$.

If we deal with a space group with a centred unit cell, the above result has to be modified slightly. If there are $k - 1$ centring vectors, the lattice spanned by the conventional basis is a sublattice of index k in the full translation lattice. The conventional cell therefore is built up from k primitive unit cells (spanned by a primitive lattice basis) and thus in particular contains k times as many points as the primitive cell (see Chapter 1.3 for a detailed discussion of conventional and primitive bases and cells).

Proposition

Let $\mathcal{G}$ be a space group with point group $\mathcal{P}$ and let $\mathcal{S}_X$ be the site-symmetry group of a point X in $\mathbb{E}^3$. Then the number of orbit points of the orbit of X which lie in a conventional cell for $\mathcal{G}$ is equal to the product $k \times |\mathcal{P}|/|\mathcal{S}_X|$, where k is the volume of the conventional cell divided by the volume of a primitive unit cell.

1.4.4.2. Wyckoff positions

As already mentioned, one of the first issues in the analysis of crystal structures is the determination of the actual atom positions. Energetically favourable configurations in inorganic compounds are often achieved when the atoms occupy positions that have a nontrivial site-symmetry group. This suggests that one should classify the points in $\mathbb{E}^3$ into equivalence classes according to their site-symmetry groups.

Definition

A point $X \in \mathbb{E}^3$ is called a point in a *general position* for the space group $\mathcal{G}$ if its site-symmetry group contains only the identity element of $\mathcal{G}$. Otherwise, X is called a point in a *special position*.

The distinctive feature of a point in a general position is that the points in its orbit are in one-to-one correspondence with the symmetry operations of the group $\mathcal{G}$ by associating the orbit point $g(X)$ with the group operation g. For different group elements g and g', the orbit points $g(X)$ and $g'(X)$ must be different, since otherwise $g^{-1}g'$ would be a non-trivial operation in the site-symmetry group of X. Therefore, the entries listed in the space-group tables for the general positions can not only be interpreted as a shorthand notation for the symmetry operations in $\mathcal{G}$ (as seen in Section 1.4.2.3), but also as coordinates of the points in the orbit of a point X in a general position with coordinates x, y, z (up to translations).

Whereas points in general positions exist for every space group, not every space group has points in a special position. Such groups are called *fixed-point-free space groups* or *Bieberbach groups* and are precisely those groups that may contain glide reflections or screw rotations, but no proper reflections, rotations, inversions and rotoinversions.

Example

The group $\mathcal{G}$ of type $Pna2_1$ (33) has a point group of order 4 and representatives for the non-trivial cosets relative to the translation subgroup are the twofold screw rotation $\bar{x}, \bar{y}, z + \frac{1}{2}$, the a glide $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ and the n glide $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$. No operation in the coset of the twofold screw rotation can have a fixed point, since such an operation maps the z component to $z + \frac{1}{2} + t_z$ for an integer t_z, and this is never equal to z. The same argument applies to the x component of the a glide and to the y component of the n glide, hence this group contains no operation with a fixed point (apart from the identity element) and is thus a fixed-point-free space group.

The distinction into general and special positions is of course very coarse. In a finer classification, it is certainly desirable that two points in the same orbit under the space group belong to the same class, since they are symmetry equivalent. Such points have *conjugate* site-symmetry groups (*cf.* the orbit–stabilizer theorem in Section 1.1.7).

Lemma

Let X and Y be points in the same orbit of a space group $\mathcal{G}$ and let $g \in \mathcal{G}$ such that $g(X) = Y$. Then the site-symmetry groups of X and Y are conjugate by the operation mapping X to Y, *i.e.* one has $\mathcal{S}_Y = g \cdot \mathcal{S}_X \cdot g^{-1}$.

The classification motivated by the conjugacy relation between the site-symmetry groups of points in the same orbit is the classification into *Wyckoff positions*.

Definition

Two points X and Y in $\mathbb{E}^3$ belong to the same *Wyckoff position* with respect to $\mathcal{G}$ if their site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of $\mathcal{G}$.

In particular, the Wyckoff position containing a point X also contains the full orbit $\mathcal{G}(X)$ of X under $\mathcal{G}$.

Remark: It is built into the definition of Wyckoff positions that points that are related by a symmetry operation of $\mathcal{G}$ belong to the same Wyckoff position. However, a single site-symmetry group may have more than one fixed point, *e.g.* points on the same rotation axis or in the same reflection plane. These points are in general not symmetry related but, having identical site-symmetry groups, clearly belong to the same Wyckoff position. This situation can be analyzed more explicitly:

Let $\mathcal{S}_X$ be the site-symmetry group of the point X and assume that Y is another point with the same site-symmetry group $\mathcal{S}_Y = \mathcal{S}_X$. Choosing a coordinate system with origin X, the operations in $\mathcal{S}_X$ all have translational part equal to zero and are thus matrix–column pairs of the form $(\boldsymbol{W}, \boldsymbol{o})$. In particular, these operations are *linear* operations, and since both points X and Y are fixed by all operations in $\mathcal{S}_X$, the vector $\mathbf{v} = Y - X$ is also fixed by the linear operations $(\boldsymbol{W}, \boldsymbol{o})$ in $\mathcal{S}_X$. But with the vector $\mathbf{v}$ each scaling $c \cdot \mathbf{v}$ of $\mathbf{v}$ is fixed as well, and therefore all the points on the line through X and Y are fixed by the operations in $\mathcal{S}_X$. This shows that the Wyckoff position of X is a union of infinitely many orbits if $\mathcal{S}_X$ has more than one fixed point.

Lemma

Let $\mathcal{S}_X$ be the site-symmetry group of X in $\mathcal{G}$:

(i) The points belonging to the same Wyckoff position as X are precisely the points in the orbit of X under $\mathcal{G}$ if and only if X is the only point fixed by all operations in $\mathcal{S}_X$. In this case the coordinates of a point belonging to this Wyckoff position have fixed values not depending on a parameter.

(ii) If Y is a further point fixed by all operations in $\mathcal{S}_X$ but there is no fixed point of $\mathcal{S}_X$ outside the line through X and Y, then all the points on the line through X and Y are fixed by $\mathcal{S}_X$. The Wyckoff position of X is then the union of the orbits of points on this line (with the exception of a possibly empty discrete subset of points which have a larger site-symmetry group). In this case the coordinates of a point belonging to this Wyckoff position have values depending on a single variable parameter.

(iii) If Y and Z are points fixed by all operations in $\mathcal{S}_X$ such that X, Y, Z do not lie on a line, then all the points on the plane through X, Y and Z are fixed by $\mathcal{S}_X$. The Wyckoff position of X is then the union of the orbits of points in this plane with the exception of a (possibly empty) discrete subset of lines or points which have a larger site-symmetry group. In this case the coordinates of a point belonging to this Wyckoff position have values depending on two variable parameters.

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$

Figure 1.4.4.1
General-position block as given in the space-group tables for space group *P*4*bm* (100).

(iv) Only the points belonging to the general position depend on three variable parameters.

The space-group tables of Chapter 2.3 contain the following information about the Wyckoff positions of a space group $\mathcal{G}$:

Multiplicity: The Wyckoff multiplicity is the number of points in an orbit for this Wyckoff position which lie in the conventional cell. For a group with a primitive unit cell, the multiplicity for the general position equals the order of the point group of $\mathcal{G}$, while for a centred cell this is multiplied by the quotient of the volumes of the conventional cell and a primitive unit cell.

The quotient of the multiplicity for the general position by that of a special position gives the order of the site-symmetry group of the special position.

Wyckoff letter: Each Wyckoff position is labelled by a letter in alphabetical order, starting with '*a*' for a position with site-symmetry group of maximal order and ending with the highest letter (corresponding to the number of different Wyckoff positions) for the general position.

It is common to specify a Wyckoff position by its multiplicity and Wyckoff letter, *e.g.* by 4*a* for a position with multiplicity 4 and letter *a*.

Site symmetry: The point group isomorphic to the site-symmetry group is indicated by an *oriented symbol*, which is a variation of the Hermann–Mauguin point-group symbol that provides information about the orientation of the symmetry elements. The constituents of the oriented symbol are ordered according to the symmetry directions of the corresponding crystal lattice (primary, secondary and tertiary). A symmetry operation in the site-symmetry group gives rise to a symbol in the position corresponding to the direction of its geometric element. Directions for which no symmetry operation contributes to the site-symmetry group are represented by a dot in the oriented symbol.

Coordinates: Under this heading, the coordinates of the points in an orbit belonging to the Wyckoff position are given, possibly depending on one or two variable parameters (three for the general position). The points given represent the orbit up to translations from the full translational subgroup. For a space group with a centred lattice, centring vectors which are coset representatives for the translation lattice relative to the lattice spanned by the conventional basis are given at the top of the table. To obtain representatives of the orbit up to translations from the lattice spanned by the conventional basis, these centring vectors have to be added to each of the given points.

As already mentioned, the coordinates given for the general position can also be interpreted as a compact notation for the symmetry operations, specified up to translations.

The entries in the last column, the *reflection conditions*, are discussed in detail in Chapter 1.6. This column lists the conditions for the reflection indices *hkl* for which the corresponding structure factor is not systematically zero.

Examples

(1) Let $\mathcal{G}$ be the space group of type *Pbca* (61) generated by the twofold screw rotations $\{2_{001}|\frac{1}{2},0,\frac{1}{2}\}$: $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$ and $\{2_{010}|0,\frac{1}{2},\frac{1}{2}\}$: $\bar{x}, y+\frac{1}{2}, \bar{z}+\frac{1}{2}$, the inversion $\{\bar{1}|0\}$: $\bar{x},\bar{y},\bar{z}$ and the translations $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$.
Applying the eight coset representatives of $\mathcal{G}$ with respect to the translation subgroup, the points in the orbit of the origin $X_1 = \begin{pmatrix}0\\0\\0\end{pmatrix}$ that lie in the unit cell are found to be X_1, $X_2 = \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$, $X_3 = \begin{pmatrix}0\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$ and $X_4 = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix}$, and the Wyckoff position to which X_1 belongs has multiplicity 4 and is labelled 4*a*.
Since the point group $\mathcal{P}$ of $\mathcal{G}$ has order 8, the site-symmetry group $\mathcal{S}_{X_1}$ has order 8/4 = 2. The inversion in the origin X_1 obviously fixes X_1, hence $\mathcal{S}_{X_1} = \{\{1|0\},\{\bar{1}|0\}\}$. The oriented symbol for the site symmetry is $\bar{1}$, indicating that the site-symmetry group is generated by an inversion.
The points X_2, X_3 and X_4 belong to the same Wyckoff position as X_1, since they lie in the orbit of X_1 and thus have conjugate site-symmetry groups.
The point $Y_1 = \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix}$ also has an orbit with 4 points in the unit cell, namely Y_1, $Y_2 = \begin{pmatrix}\frac{1}{2}\\0\\0\end{pmatrix}$, $Y_3 = \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$ and $Y_4 = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$. These points therefore belong to a common Wyckoff position, namely position 4*b*. Moreover, the site-symmetry group of Y_1 is also generated by an inversion, namely the inversion $\{\bar{1}|0,0,1\}$: $\bar{x},\bar{y},\bar{z}+1$ located at Y_1 and is thus denoted by the oriented symbol $\bar{1}$.
The points X_1 and Y_1 do not belong to the same Wyckoff position, because an operation $(\boldsymbol{W},\boldsymbol{w})$ in $\mathcal{G}$ conjugates the inversion $\{\bar{1}|0,0,0\}$ in the origin to an inversion in $\boldsymbol{w}$. Since the translational parts of the operations in $\mathcal{G}$ are (up to integers) $(0,0,0)$, $(\frac{1}{2},\frac{1}{2},0)$, $(\frac{1}{2},0,\frac{1}{2})$ and $(0,\frac{1}{2},\frac{1}{2})$, an inversion in $Y_1 = \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix}$ can not be obtained by conjugation with operations from $\mathcal{G}$.

(2) Let $\mathcal{G}$ be the space group of type *P*4*bm* (100) generated by the fourfold rotation $\{4^+|0\}$: $\bar{y}, x, z$, the glide reflection (of *b* type) $\{m_{100}|\frac{1}{2},\frac{1}{2},0\}$: $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, z$ and the translations $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$. The general-position coordinate triplets are shown in Fig. 1.4.4.1
From this information, the coordinates for the orbit of a specific point X in a special position can be derived by simply inserting the coordinates of X into the general-

position coordinates, normalizing to values between 0 and 1 (by adding ±1 if required) and eliminating duplicates.

For example, for the point $X = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{4} \end{pmatrix}$ in Wyckoff position 2b one obtains X and $Y = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}$ as the points in the orbit of X that lie in the unit cell. Since the point group $\mathcal{P}$ of $\mathcal{G}$ has order 8, the site-symmetry group $\mathcal{S}_X$ is a group of order 8/2 = 4. Its four operations are

Coordinate triplet	Description
x, y, z	Identity operation
$\bar{x}+1, \bar{y}, z$	Twofold rotation with axis $\frac{1}{2}, 0, z$
$\bar{y}+\frac{1}{2}, \bar{x}+\frac{1}{2}, z$	Reflection with plane $x+\frac{1}{2}, -x, z$
$y+\frac{1}{2}, x-\frac{1}{2}, z$	Reflection with plane $x+\frac{1}{2}, x, z$

The corresponding oriented symbol for the site-symmetry is 2.*mm*, indicating that the site-symmetry group contains a twofold rotation along a primary lattice direction, no symmetry operations along the secondary directions and two reflections along tertiary directions.

Since X and Y lie in the same orbit, they clearly belong to the same Wyckoff position. But every point $X' = \begin{pmatrix} \frac{1}{2} \\ 0 \\ z \end{pmatrix}$ with $0 \le z < 1$ has the same site-symmetry group as X and therefore also belongs to the same Wyckoff position as X. Inserting the coordinates of X' in the general-position coordinates, one obtains $Y' = \begin{pmatrix} 0 \\ \frac{1}{2} \\ z \end{pmatrix}$ as the only other point in the orbit of X' that lies in the unit cell. Clearly, Y' has the same site-symmetry group as Y. The Wyckoff position 2b to which X belongs therefore consists of the union of the orbits of the points $X' = \begin{pmatrix} \frac{1}{2} \\ 0 \\ z \end{pmatrix}$ with $0 \le z < 1$.

In the space-group diagram in Fig. 1.4.4.2, the points belonging to Wyckoff position 2b can be identified as the points on the intersection of a twofold rotation axis directed along [001] and two reflection planes normal to the square diagonals and crossing the centres of the sides bordering the unit cell. It is clear that for every value of z, the four intersection points in the unit cell lie in one orbit under the fourfold rotation located in the centre of the displayed cell.

Applying the same procedure to a point $X = \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}$ in Wyckoff position 2a, the points in the orbit that lie in the unit cell are seen to be X and $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ z \end{pmatrix}$. The site-symmetry group $\mathcal{S}_X$ is again of order 4 and since the fourfold rotation $\{4^+|0\}$ fixes X, $\mathcal{S}_X$ is the cyclic group of order 4 generated by this fourfold rotation. The oriented symbol for this site-symmetry group is 4.. and the corresponding points can easily be identified in the space-group diagram in Fig. 1.4.4.2 by the symbol for a fourfold rotation.

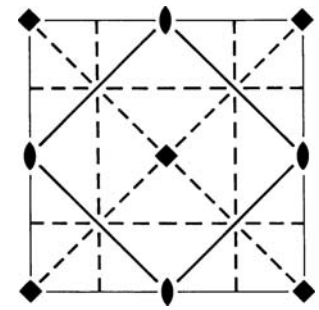

Figure 1.4.4.2
Symmetry-element diagram for the space group *P*4*bm* (100) for the orthogonal projection along [001].

Since a point in a special position has to lie on the geometric element of a reflection, rotation or inversion, the special positions can in principle be read off from the space-group diagrams. In the present example, we have dealt with the positions fixed by twofold or fourfold rotations, and from the diagram in Fig. 1.4.4.2 one sees that the only remaining case is that of points on reflection planes, indicated by the solid lines. A point on such a reflection plane is $X = \begin{pmatrix} x \\ x+\frac{1}{2} \\ z \end{pmatrix}$ and by inserting these coordinates into the general-position coordinates one obtains the points $\bar{x}, \bar{x}+\frac{1}{2}, z$, $\bar{x}+\frac{1}{2}, x, z$ and $x+\frac{1}{2}, \bar{x}, z$ as the other points in the orbit of X (up to translations). Here, the site-symmetry group $\mathcal{S}_X$ is of order 2, it is generated by the reflection $\{m_{1\bar{1}0}|-\frac{1}{2},\frac{1}{2},0\}$: $y-\frac{1}{2}, x+\frac{1}{2}, z$ having the plane $x, x+\frac{1}{2}, z$ as geometric element. The oriented symbol of $\mathcal{S}_X$ is ..*m*, since the reflection is along a tertiary direction.

1.4.4.3. Wyckoff sets

Points belonging to the same Wyckoff position have conjugate site-symmetry groups and thus in particular all those points are collected together that lie in one orbit under the space group $\mathcal{G}$. However, in addition, points that are not symmetry-related by a symmetry operation in $\mathcal{G}$ may still play geometrically equivalent roles, *e.g.* as intersections of rotation axes with certain reflection planes.

Example

In the conventional setting, the fourfold axes of a space group $\mathcal{G}$ of type *P*4 (75) intersect the *ab* plane in the points $u_1, u_2, 0$ and $u_1+\frac{1}{2}, u_2+\frac{1}{2}, 0$ for integers u_1, u_2, as can be seen from the space-group diagram in Fig. 1.4.4.3.

The points $u_1, u_2, 0$ lie in one orbit under the translation subgroup of $\mathcal{G}$, and thus belong to the same Wyckoff position, labelled 1a. For the same reason, the points $u_1+\frac{1}{2}, u_2+\frac{1}{2}, 0$ belong to a single Wyckoff position, namely to position 1b. The points $X = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ and $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ do not belong to the same Wyckoff position, because the site-symmetry group $\mathcal{S}_X$ is generated by the fourfold rotation 4_{001} and conjugating this by an operation $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$ results in a fourfold rotation with axis parallel to the c axis and running through $\boldsymbol{w}$. But since the translation parts of all operations in $\mathcal{G}$ are integral, such an axis

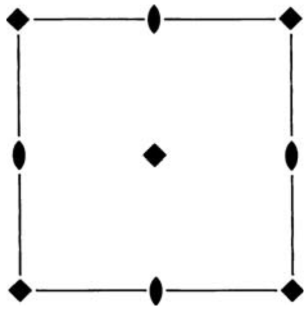

Figure 1.4.4.3
Symmetry-element diagram for the space group *P*4 (75) for the orthogonal projection along [001].

can not contain $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and thus $\mathcal{S}_X$ and $\mathcal{S}_Y$ are not conjugate in $\mathcal{G}$.
However, the translation by $(\frac{1}{2}, \frac{1}{2}, 0)$ conjugates $\mathcal{S}_X$ to $\mathcal{S}_Y$, while fixing the group $\mathcal{G}$ as a whole. This shows that there is an ambiguity in choosing the origin either at 0, 0, 0 or $\frac{1}{2}, \frac{1}{2}, 0$, since these points are geometrically indistinguishable (both being intersections of a fourfold axis with the *ab* plane).

The ambiguity in the origin choice in the above example can be explained by the *affine normalizer* of the space group $\mathcal{G}$ (see Section 1.1.8 for a general introduction to normalizers). The full group $\mathcal{A}$ of affine mappings acts *via* conjugation on the set of space groups and the space groups of the same affine type are obtained as the orbit of a single group of that type under $\mathcal{A}$.

Definition
The group $\mathcal{N}$ of affine mappings $n \in \mathcal{A}$ that fix a space group $\mathcal{G}$ under conjugation is called the *affine normalizer* of $\mathcal{G}$, *i.e.*

$$\mathcal{N} = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = \{n \in \mathcal{A} | n\mathcal{G}n^{-1} = \mathcal{G}\}.$$

The affine normalizer is the largest subgroup of $\mathcal{A}$ such that $\mathcal{G}$ is a normal subgroup of $\mathcal{N}$.

Conjugation by operations of the affine normalizer results in a permutation of the operations of $\mathcal{G}$, *i.e.* in a relabelling without changing their geometric properties. The additional translations contained in the affine normalizer can in fact be derived from the space-group diagrams, because shifting the origin by such a translation results in precisely the same diagram. More generally, an element of the affine normalizer can be interpreted as a change of the coordinate system that does not alter the space-group diagrams.

A more thorough description of the affine normalizers of space groups is given in Chapter 3.5, where tables with the affine normalizers are also provided.

Since the affine normalizer of a space group $\mathcal{G}$ is in general a group containing $\mathcal{G}$ as a proper subgroup, it is possible that subgroups of $\mathcal{G}$ that are not conjugate by any operation of $\mathcal{G}$ may be conjugate by an operation in the affine normalizer. As a consequence, the site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ of two points X and Y belonging to different Wyckoff positions of $\mathcal{G}$ may be conjugate under the affine normalizer of $\mathcal{G}$. This reveals that the points X and Y are in fact geometrically equivalent, since they fall into the same orbit under the affine normalizer of $\mathcal{G}$. Joining the equivalence classes of these points into a single class results in a coarser classification with larger classes, which are called *Wyckoff sets*.

Definition
Two points X and Y belong to the same *Wyckoff set* if their site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of the affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of $\mathcal{G}$.
In particular, the Wyckoff set containing a point X also contains the full orbit of X under the affine normalizer of $\mathcal{G}$.

Example
Let $\mathcal{G}$ be the space group of type $P222_1$ (17) generated by the translations of an orthorhombic lattice, the twofold rotation $\{2_{100}|0\}$: $x, \bar{y}, \bar{z}$ and the twofold screw rotation $\{2_{001}|0, 0, \frac{1}{2}\}$: $\bar{x}, \bar{y}, z + \frac{1}{2}$. Note that the composition of these two elements is the twofold rotation with the line $0, y, \frac{1}{4}$ as its geometric element. The group $\mathcal{G}$ has four different Wyckoff positions with a site-symmetry group generated by a twofold rotation; representatives of these Wyckoff positions are the points $X_1 = \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix}$ (Wyckoff position 2*a*, site-symmetry symbol 2..), $X_2 = \begin{pmatrix} x \\ \frac{1}{2} \\ 0 \end{pmatrix}$ (position 2*b*, symbol 2..), $Y_1 = \begin{pmatrix} 0 \\ y \\ \frac{1}{4} \end{pmatrix}$ (position 2*c*, symbol .2.) and $Y_2 = \begin{pmatrix} \frac{1}{2} \\ y \\ \frac{1}{4} \end{pmatrix}$ (position 2*d*, symbol .2.).
From the tables of affine normalizers in Chapter 3.5, but also by a careful analysis of the space-group diagrams in Fig. 1.4.4.4, one deduces that the affine normalizer of $\mathcal{G}$ contains the additional translations $t(\frac{1}{2}, 0, 0)$, $t(0, \frac{1}{2}, 0)$ and $t(0, 0, \frac{1}{2})$, since all the diagrams are invariant by a shift of $\frac{1}{2}$ along any of the coordinate axes. Moreover, the symmetry operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$: $y, x, z + \frac{1}{4}$ which interchanges the *a* and *b* axes and shifts the origin by $\frac{1}{4}$ along the *c* axis belongs to the affine

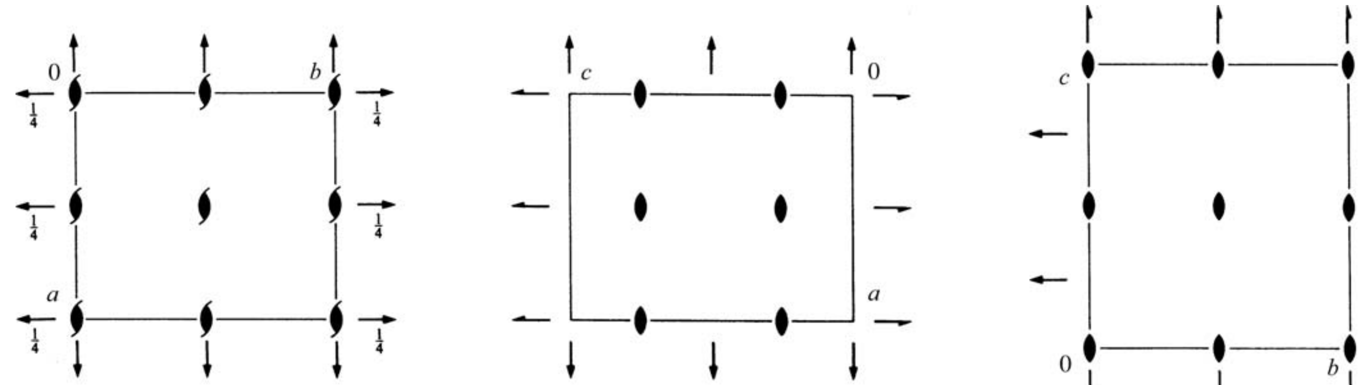

Figure 1.4.4.4
Symmetry-element diagrams for the space group $P222_1$ (17) for orthogonal projections along [001], [010], [100] (left to right).

normalizer, because it precisely interchanges the twofold rotations around axes parallel to the a and to the b axes. The translation $t(0, \frac{1}{2}, 0)$ maps X_1 to X_2, and hence X_1 and X_2 have site-symmetry groups which are conjugate under the affine normalizer of $\mathcal{G}$ and thus belong to the same Wyckoff set. Analogously, Y_1 and Y_2 belong to the same Wyckoff set, because $t(\frac{1}{2}, 0, 0)$ maps Y_1 to Y_2. Finally, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ found in the affine normalizer maps X_1 to Y_1. This shows that the points of all four Wyckoff positions actually belong to the same Wyckoff set.

Geometrically, the positions in this Wyckoff set can be described as those points that lie on a twofold rotation axis.

The assignments of Wyckoff positions of plane and space groups to Wyckoff sets are discussed and tabulated in Chapter 3.4.

Remark: The previous example deserves some further discussion. The group $\mathcal{G}$ of type $P222_1$ belongs to the orthorhombic crystal family, and the conventional unit cell is spanned by three basis vectors **a**, **b**, **c** with lengths a, b, c and right angles between each pair of basis vectors. Unless the parameters a and b are equal because of some metric specialization, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ of the affine normalizer is not an isometry but changes lengths. If it is desired that the metric properties are preserved, the full affine normalizer cannot be taken into account, but only the subgroup that consists of isometries. This subgroup is called the *Euclidean normalizer* of $\mathcal{G}$. (A detailed discussion of Euclidean normalizers of space groups and their tabulation are given in Chapter 3.5.)

Taking conjugacy of the site-symmetry groups under the Euclidean normalizer as a condition results in a notion of equivalence which lies between that of Wyckoff positions and Wyckoff sets. In the above example, the four Wyckoff positions would be merged into two classes represented by X_1 and Y_1, but X_1 and Y_1 would not be regarded as equivalent, since they are not related by an operation of the Euclidean normalizer.

It turns out, however, that in many cases this intermediate classification coincides with the Wyckoff sets, because points belonging to different Wyckoff positions are often related to each other by a translation contained in the affine normalizer. Since translations are always isometries, the translations contained in the affine normalizer always belong to the Euclidean normalizer as well.

1.4.4.4. Eigensymmetry groups and non-characteristic orbits

A crystallographic orbit $\mathcal{O}$ has been defined as the set of points $g(X)$ obtained by applying all operations of some space group $\mathcal{G}$ to a point $X \in \mathbb{E}^3$. From that it is clear that the set $\mathcal{O}$ is invariant as a whole under the action of operations in $\mathcal{G}$, since for some point $Y = g(X)$ in the orbit and $h \in \mathcal{G}$ one has $h(Y) = (hg)(X)$, which is again contained in $\mathcal{O}$ because hg belongs to $\mathcal{G}$. However, it is possible that the orbit $\mathcal{O}$ is also invariant under some isometries of $\mathbb{E}^3$ that are not contained in $\mathcal{G}$. Since the composition of two such isometries still keeps the orbit invariant, the set of all isometries leaving $\mathcal{O}$ invariant forms a group which contains $\mathcal{G}$ as a subgroup.

Definition

Let $\mathcal{O} = \{g(X)|g \in \mathcal{G}\}$ be the orbit of a point $X \in \mathbb{E}^3$ under a space group $\mathcal{G}$. Then the group $\mathcal{E}$ of isometries of $\mathbb{E}^3$ which leave $\mathcal{O}$ invariant as a whole is called the *eigensymmetry group* of $\mathcal{O}$.

Since the orbit is a discrete set, the eigensymmetry group has to be a space group itself. One distinguishes the following cases:

(i) The eigensymmetry group $\mathcal{E}$ equals the group $\mathcal{G}$ by which the orbit was generated. In this case the orbit is called a *characteristic orbit* of $\mathcal{G}$.

(ii) The eigensymmetry group $\mathcal{E}$ contains $\mathcal{G}$ as a proper subgroup. Then the orbit is called a *non-characteristic orbit*.

(iii) If the eigensymmetry group $\mathcal{E}$ contains translations that are not contained in $\mathcal{G}$, *i.e.* if $\mathcal{T}_{\mathcal{G}}$ is a proper subgroup of $\mathcal{T}_{\mathcal{E}}$, the orbit is called an *extraordinary orbit*. Of course, extraordinary orbits are a special kind of non-characteristic orbits.

Non-characteristic orbits are closely related to the concept of *lattice complexes*, which are discussed in Chapter 3.4. An extensive listing of non-characteristic orbits of space groups can be found in Engel *et al.* (1984).

The fact that an orbit of a space group has a larger eigensymmetry group is an important example of a pair of groups that are in a group–subgroup relation. Knowledge of subgroups and supergroups of a given space group play a crucial role in the analysis of phase transitions, for example, and are discussed in detail in Chapter 1.7.

The occurrence of non-characteristic orbits does not require the point X to be chosen at a special position. Even the general position of a space group $\mathcal{G}$ may give rise to a non-characteristic orbit. Moreover, special values of the coordinates of the general position may give rise to additional eigensymmetries without the position becoming a special position. Conversely, the orbit of a point at a special position need not be non-characteristic.

Example

We compare space groups of types $P4_1$ (76) and $P4_2$ (77). For a space group of type $P4_1$, the general position with generic coordinates x, y, z gives rise to a characteristic orbit, whereas the general-position orbit for a space group of type $P4_2$ consists of the points $X_1 = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, $X_2 = \begin{pmatrix} \bar{x} \\ \bar{y} \\ z \end{pmatrix}$, $X_3 = \begin{pmatrix} \bar{y} \\ x \\ z+\frac{1}{2} \end{pmatrix}$ and $X_4 = \begin{pmatrix} y \\ \bar{x} \\ z+\frac{1}{2} \end{pmatrix}$. An inversion $\{\bar{1}|0, 0, 2z\}$ in $0, 0, z$ interchanges X_1 and X_2, and maps X_3 to $y, \bar{x}, z-\frac{1}{2}$, which is clearly equivalent to X_4 under a translation. This shows that the general-position orbit for a space group of type $P4_2$ is a non-characteristic orbit, and the eigensymmetry group of this orbit is of type $P4_2/m$ (84), where the origin has to be shifted to the inversion point $0, 0, z$ to obtain the conventional setting. Since the unit cell and the orbit are unchanged, but the point group of $P4_2$ is a subgroup of index 2 in the point group of $P4_2/m$, the orbit points must belong to a special position for $P4_2/m$, namely the position labelled $4j$. In the conventional setting of $P4_2/m$, a point belonging to this Wyckoff position is given by x, y, 0 and one finds that the orbit of this point in special position is characteristic, *i.e.* its eigensymmetry group is just $P4_2/m$.

If we assume that the metric of the space group is not special, the eigensymmetry group is restricted to the same crystal family (for the definition of 'specialized' metrics, *cf.* Section 1.3.4.3 and Chapter 3.5). Therefore, a space group $\mathcal{G}$ for which the point group is a holohedry can only have non-characteristic orbits by additional translations, *i.e.* extraordinary orbits. However, if we allow specialized metrics, the eigensymmetry group may belong to a higher crystal family. For example, if a space group belongs to the orthorhombic family, but the unit cell has equal parameters

$a = b$, then the eigensymmetry group of an orbit can belong to the tetragonal family.

Note: A space group $\mathcal{G}$ is equal to the intersection of the eigensymmetry groups of the orbits of all its positions. If none of the positions of a space group $\mathcal{G}$ gives rise to a characteristic orbit, this means that each single orbit under $\mathcal{G}$ does not have $\mathcal{G}$ as its symmetry group, but a larger group that contains $\mathcal{G}$ as a proper subgroup. It may thus be necessary to have the union of at least two orbits under $\mathcal{G}$ to obtain a structure that has precisely $\mathcal{G}$ as its group of symmetry operations.

Examples

(1) For the group $\mathcal{G}$ of type *Pmmm* (47) all Wyckoff positions with no further special values of the coordinates give rise to characteristic orbits, because the point group of $\mathcal{G}$ is a holohedry and the general coordinates allow no further translations. However, there are various 'specializations' of the positions that give rise to extraordinary orbits. For example, setting x to the special value $\frac{1}{4}$ for the general position introduces the additional translation $t(\frac{1}{2}, 0, 0)$. In fact, for all positions in which the first coordinate has no specified value (positions 2*i*–2*l*, 4*w*–4*z*, 8α), setting $x = \frac{1}{4}$ introduces the translation $t(\frac{1}{2}, 0, 0)$ and thus gives rise to an extraordinary orbit. In all these cases, the resulting eigensymmetry group is of type *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}, \mathbf{b}, \mathbf{c}$.

(2) For the group $\mathcal{G}$ of type *Pmm*2 (25) no Wyckoff position gives rise to a characteristic orbit, because this is a polar group (with respect to the *c* axis). Any orbit of a point with third coordinate z allows an additional mirror plane normal to the *c* axis and located at $0, 0, z$. For example, the general position gives rise to a non-characteristic orbit with eigensymmetry group *Pmmm* (47). Since the general coordinates allow no additional translation, this is not an extraordinary orbit. However, setting $x = \frac{1}{4}$ for the general position introduces the translation $t(\frac{1}{2}, 0, 0)$ (as in the above example) and thus gives rise to an extraordinary orbit. The eigensymmetry group is *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}, \mathbf{b}, \mathbf{c}$.

On the other hand, the special positions $x, 0, z$ (Wyckoff position 2*e*) and $x, \frac{1}{2}, z$ (Wyckoff position 2*f*) both have the same eigensymmetry group as the general position and setting $x = \frac{1}{4}$ for each, giving $\frac{1}{4}, 0, z$ and $\frac{1}{4}, \frac{1}{2}, z$, results in these positions having the same eigensymmetry group as the $\frac{1}{4}, y, z$ case of the general position.

(3) For a group $\mathcal{G}$ of type $P\bar{4}c2$ (116) the general-position coordinates are

(1) x, y, z	(2) $\bar{x}, \bar{y}, z$	(3) $y, \bar{x}, \bar{z}$	(4) $\bar{y}, x, \bar{z}$
(5) $x, \bar{y}, z + \frac{1}{2}$	(6) $\bar{x}, y, z + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$

A point x, y, z in a general position does not give rise to an extraordinary orbit because, owing to the general coordinates, there can not be any additional translation. Furthermore, the point group $\bar{4}m2$ of $\mathcal{G}$ has index 2 in the holohedry $4/mmm$. Thus, in order to have a non-characteristic orbit one would require an inversion in some point as an additional operation. But an inversion in p_1, p_2, p_3 would map x, y, z to $\bar{x} + 2p_1, \bar{y} + 2p_2, \bar{z} + 2p_3$ and no such point is contained in the orbit for generic x, y, z. The point x, y, z therefore gives rise to a characteristic orbit.

However, if the point in a general position is chosen with $x = y$, one indeed obtains an additional inversion at $0, 0, \frac{1}{4}$ which maps x, x, z to the orbit point $\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$ (general position point No. 8). This orbit thus is non-characteristic, but it is not extraordinary, since no additional translation is introduced. The eigensymmetry group obtained is $P4_2/mcm$ (132).

On the other hand, if the general position is chosen with $y = 0$, no additional inversion is obtained, but the translation by $\frac{1}{2}\mathbf{c}$ maps $x, 0, z$ to $x, 0, z + \frac{1}{2}$ (general-position point No. 5). The position $x, 0, z$ therefore gives rise to an extraordinary orbit with eigensymmetry group $P\bar{4}m2$ (115).

Knowledge of the eigensymmetry groups of the different positions for a group is of utmost importance for the analysis of diffraction patterns. Atoms in positions that give rise to non-characteristic orbits, in particular extraordinary orbits, may cause systematic absences that are not explained by the space-group operations. These absences are specified as *special reflection conditions* in the space-group tables of this volume, but only as long as no specialization of the coordinates is involved. For the latter case, the possible existence of systematic absences has to be deduced from the tables of noncharacteristic orbits. Reflection conditions are discussed in detail in Chapter 1.6.

Example

For the group $\mathcal{G}$ of type *Pccm* (49) the special position $\frac{1}{2}, 0, z$ (Wyckoff position 4*p*) gives rise to an extraordinary orbit, since it allows the additional translation $\frac{1}{2}\mathbf{c}$. The special reflection condition corresponding to this additional translation is the integral reflection condition *hkl*: $l = 2n$. However, if the z coordinate in position 4*p* is set to $z = \frac{1}{8}$, the eigensymmetry group also contains the translation $\frac{1}{4}\mathbf{c}$. In this case, the special reflection condition becomes *hkl*: $l = 4n$.

1.4.5. Sections and projections of space groups

BY B. SOUVIGNIER

In crystallography, two-dimensional sections and projections of crystal structures play an important role, *e.g.* in structure determination by Fourier and Patterson methods or in the treatment of twin boundaries and domain walls. Planar sections of three-dimensional scattering density functions are used for finding approximate locations of atoms in a crystal structure. They are indispensable for the location of Patterson peaks corresponding to vectors between equivalent atoms in different asymmetric units (the Harker vectors).

1.4.5.1. Introduction

A two-dimensional section of a crystal pattern takes out a slice of a crystal pattern. In the mathematical idealization, this slice is regarded as a two-dimensional plane, allowing one, however, to distinguish its upper and lower side. Depending on how the slice is oriented with respect to the crystal lattice, the slice will be invariant by translations of the crystal pattern along zero, one or two linearly independent directions. A section resulting in a slice with two-dimensional translational symmetry is called a *rational section* and is by far the most important case for crystallography.

Because the slice is regarded as a two-sided plane, the symmetries of the full crystal pattern that leave the slice invariant fall into two types:

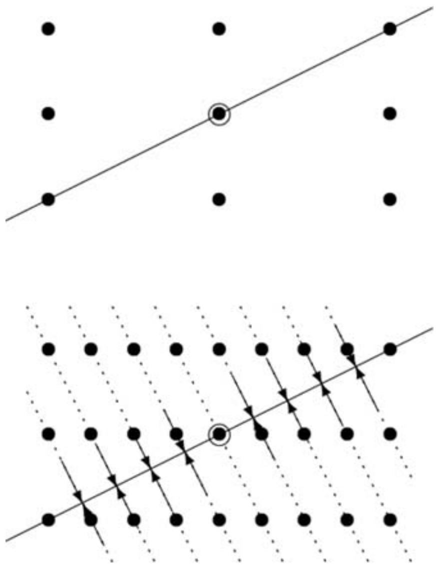

Figure 1.4.5.1
Duality between section and projection.

corresponds to a projection in direct space and *vice versa*. The projection direction in the one space is normal to the slice in the other space. This correspondence is illustrated schematically in Fig. 1.4.5.1. The top part shows a rectangular lattice with $b/a = 2$ and a slice along the line defined by $2x + y = 0$. Normalizing $a = 1$, the distance between two neighbouring lattice points in the slice is $\sqrt{5}$. If the pattern is restricted to this slice, the points of the corresponding diffraction pattern in reciprocal space must have distance $1/\sqrt{5}$ and this is precisely obtained by projecting the lattice points of the reciprocal lattice onto the slice.

The different, but related, viewpoints of sections and projections can be stated in a simple way as follows: For a section perpendicular to the c axis, only those points of a crystal pattern are considered which have z coordinate equal to a fixed value z_0 or in a small interval around z_0. For a projection along the c axis, all points of the crystal pattern are considered, but their z coordinate is simply ignored. This means that all points of the crystal pattern that differ only by their z coordinate are regarded as the same point.

(i) If a symmetry operation of the slice maps its upper side to the upper side, a vector normal to the slice is fixed.
(ii) If a symmetry operation of the slice maps the upper side to the lower side, a vector normal to the slice is mapped to its opposite and the slice is turned upside down.

Therefore, the symmetries of two-dimensional rational sections are described by *layer groups*, *i.e.* subgroups of space groups with a two-dimensional translation lattice. Layer groups are *subperiodic groups* and for their elaborate discussion we refer to Chapter 1.7 and *IT* E (2010).

Analogous to two-dimensional sections of a crystal pattern, one can also consider the penetration of crystal patterns by a straight line, which is the idealization of a one-dimensional section taking out a rod of the crystal pattern. If the penetration line is along the direction of a translational symmetry of the crystal pattern, the rod has one-dimensional translational symmetry and its group of symmetries is a *rod group*, *i.e.* a subgroup of a space group with a one-dimensional translation lattice. Rod groups are also subperiodic groups, *cf. IT* E for their detailed treatment and listing.

A projection along a direction **d** into a plane maps a point of a crystal pattern to the intersection of the plane with the line along **d** through the point. If the projection direction is not along a rational lattice direction, the projection of the crystal pattern will contain points with arbitrarily small distances and additional restrictions are required to obtain a discrete pattern (*e.g.* the cut-and-project method used in the context of quasicrystals). We avoid any such complication by assuming that **d** is along a rational lattice direction. Furthermore, one is usually only interested in *orthogonal* projections in which the projection direction is perpendicular to the projection plane. This has the effect that spheres in three-dimensional space are mapped to circles in the projection plane.

Although it is also possible to regard the projection plane as a two-sided plane by taking into account from which side of the plane a point is projected into it, this is usually not done. Therefore, the symmetries of projections are described by ordinary plane groups.

Sections and projections are related by the *projection–slice theorem* (Bracewell, 2003) of Fourier theory: A section in reciprocal space containing the origin (the so-called zero layer)

1.4.5.2. Sections

For a space group $\mathcal{G}$ and a point X in the three-dimensional point space $\mathbb{E}^3$, the site-symmetry group of X is the subgroup of operations of $\mathcal{G}$ that fix X. Analogously, one can also look at the subgroup of operations fixing a one-dimensional line or a two-dimensional plane. If the line is along a rational direction, it will be fixed at least by the translations of $\mathcal{G}$ along that direction. However, it may also be fixed by a symmetry operation that reverses the direction of the line. The resulting subgroup of $\mathcal{G}$ that fixes the line is a *rod group*.

Similarly, a plane having a normal vector along a rational direction is fixed by translations of $\mathcal{G}$ corresponding to a two-dimensional lattice. Again, the plane may also be fixed by additional symmetry operations, *e.g.* by a twofold rotation around an axis lying in the plane, by a rotation around an axis normal to the plane or by a reflection in the plane.

Definition

A *rational planar section* of a crystal pattern is the intersection of the crystal pattern with a plane containing two linearly independent translation vectors of the crystal pattern. The intersecting plane is called the *section plane*.

A *rational linear section* of a crystal pattern is the intersection of the crystal pattern with a line containing a translation vector of the crystal pattern. The intersecting line is called the *penetration line*.

A planar section is determined by a vector **d** which is perpendicular to the section plane and a continuous parameter s, called the *height*, which gives the position of the plane on the line along **d**.

A linear section is specified by a vector **d** parallel to the penetration line and a point in a plane perpendicular to **d** giving the intersection of the line with that plane.

Definition

(i) The symmetry group of a planar section of a crystal pattern is the subgroup of the space group $\mathcal{G}$ of the crystal pattern that leaves the section plane invariant as a whole.

If the section is a rational section, this symmetry group is a *layer group*, *i.e.* a subgroup of a space group which contains translations only in a two-dimensional plane.

(ii) The symmetry group of a linear section of a crystal pattern is the subgroup of the space group $\mathcal{G}$ of the crystal pattern that leaves the penetration line invariant as a whole.

If the section is a rational section, this symmetry group is a *rod group*, *i.e.* a subgroup of a space group which contains translations only along a one-dimensional line.

Table 1.4.5.1
Coset representatives of $Pmn2_1$ (31) relative to its translation subgroup

Seitz symbol	Coordinate triplet	Description
$\{1\|0\}$	x, y, z	Identity
$\{2_{001}\|\frac{1}{2}, 0, \frac{1}{2}\}$	$\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$	Twofold screw rotation with axis along [001]
$\{m_{010}\|\frac{1}{2}, 0, \frac{1}{2}\}$	$x+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$	*n*-glide reflection with normal vector along [010]
$\{m_{100}\|0\}$	$\bar{x}, y, z$	Reflection with normal vector along [100]

From now on we will only consider rational sections and omit this attribute. Moreover, we will concentrate on the case of planar sections, since this is by far the most relevant case for crystallographic applications. The treatment of one-dimensional sections is analogous, but in general much easier.

Let **d** be a vector perpendicular to the section plane. In most cases, **d** is chosen as the shortest lattice vector perpendicular to the section plane. However, in the triclinic and monoclinic crystal family this may not be possible, since the translations of the crystal pattern may not contain a vector perpendicular to the section plane. In that case, we assume that **d** captures the periodicity of the crystal pattern perpendicular to the section plane. This is achieved by choosing **d** as the shortest non-zero projection of a lattice vector to the line through the origin which is perpendicular to the section plane. Because of the periodicity of the crystal pattern along **d**, it is enough to consider heights s with $0 \le s < 1$, since for an integer m the sectional layer groups at heights s and $s + m$ are conjugate subgroups of $\mathcal{G}$. This is a consequence of the orbit–stabilizer theorem in Section 1.1.7, applied to the group $\mathcal{G}$ acting on the planes in $\mathbb{E}^3$. The layer at height s is mapped to the layer at height $s + m$ by the translation through $m\mathbf{d}$. Thus, the two layers lie in the same orbit under $\mathcal{G}$. According to the orbit–stabilizer theorem, the corresponding stabilizers, being just the layer groups at heights s and $s + m$, are then conjugate by the translation through $m\mathbf{d}$.

Since we assume a rational section, the sectional layer group will always contain translations along two independent directions $\mathbf{a}'$, $\mathbf{b}'$ which, we assume, form a crystallographic basis for the lattice of translations fixing the section plane. The points in the section plane at height s are then given by $x\mathbf{a}' + y\mathbf{b}' + s\mathbf{d}$. In order to determine whether the sectional layer group contains additional symmetry operations which are not translations, the following simple remark is crucial:

Let g be an operation of a sectional layer group. Then the rotational part of g maps **d** either to +**d** or to −**d**. In the former case, g is side-preserving, in the latter case it is side-reversing. Moreover, since the section plane remains fixed under g, the vectors $\mathbf{a}'$ and $\mathbf{b}'$ are mapped to linear combinations of $\mathbf{a}'$ and $\mathbf{b}'$ by the rotational part of g. Therefore, with respect to the (usually non-conventional) basis $\mathbf{a}'$, $\mathbf{b}'$, **d** of three-dimensional space and some choice of origin, the operation g has an augmented matrix of the form

$$\left(\begin{array}{ccc|c} r_{11} & r_{12} & 0 & t_1 \\ r_{21} & r_{22} & 0 & t_2 \\ 0 & 0 & r_{33} & t_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Here, $r_{33} = \pm 1$. Moreover, if $r_{33} = 1$, *i.e.* g is side-preserving, then t_3 is necessarily zero, since otherwise the plane is shifted along **d**. On the other hand, if $r_{33} = -1$, *i.e.* g is side-reversing, then a plane situated at height s along **d** is only fixed if $t_3 = 2s$.

From these considerations it is straightforward to determine the conditions under which a space-group operation belongs to a certain sectional layer group (excluding translations):

The side-preserving operations will belong to the sectional layer groups for all planes perpendicular to **d**, independent of the height s:

(i) rotations with axis parallel to **d**;
(ii) reflections with normal vector perpendicular to **d**;
(iii) glide reflections with normal vector and glide vector perpendicular to **d**.

Side-reversing operations will only occur in the sectional layer groups for planes at special heights along **d**:

(i) inversion with inversion point in the section plane;
(ii) twofold rotations or twofold screw rotations with rotation axis in the section plane;
(iii) reflections or glide reflections through the section plane with glide vector perpendicular to **d**;
(iv) rotoinversions with axis parallel to **d** and inversion point in the section plane.

Note that, because of the periodicity along **d**, a side-reversing operation that occurs at height s gives rise to a side-reversing operation of the same type occurring at height $s + \frac{1}{2}$: if g is a side-reversing symmetry operation fixing a layer at height s, then g maps a point in the layer at height $s + \frac{1}{2}$ with coordinates $x, y, s + \frac{1}{2}$ (with respect to the layer-adapted basis $\mathbf{a}'$, $\mathbf{b}'$, **d**) to a point with coordinates $x', y', s - \frac{1}{2}$ and hence the composition $t_{\mathbf{d}}g$ of g with the translation by **d** maps $x, y, s + \frac{1}{2}$ to $x', y', s + \frac{1}{2}$, *i.e.* it fixes the layer at height $s + \frac{1}{2}$. This shows that the composition with the translation by **d** provides a one-to-one correspondence between the side-reversing symmetry operations in the layer group at height s with those at height $s + \frac{1}{2}$.

If a section allows any side-reversing symmetry at all, then the side-preserving symmetries of the section form a subgroup of index 2 in the sectional layer group. Since the side-preserving symmetries exist independently of the height parameter s, the full sectional layer group is always generated by the side-preserving subgroup and either none or a single side-reversing symmetry.

Summarizing, one can conclude that for a given space group the interesting sections are those for which the perpendicular vector **d** is parallel or perpendicular to a symmetry direction of the group, *e.g.* an axis of a rotation or rotoinversion or the normal vector of a reflection or glide reflection.

Example

Consider the space group $\mathcal{G}$ of type $Pmn2_1$ (31). In its standard setting, the cosets of $\mathcal{G}$ relative to the translation subgroup are represented by the operations given in Table 1.4.5.1.

Since this is an orthorhombic group, it is natural to consider sections along the coordinate axes. The space-group diagrams displayed in Fig. 1.4.5.2, which show the orthogonal projections of the symmetry elements along these directions, are very helpful.

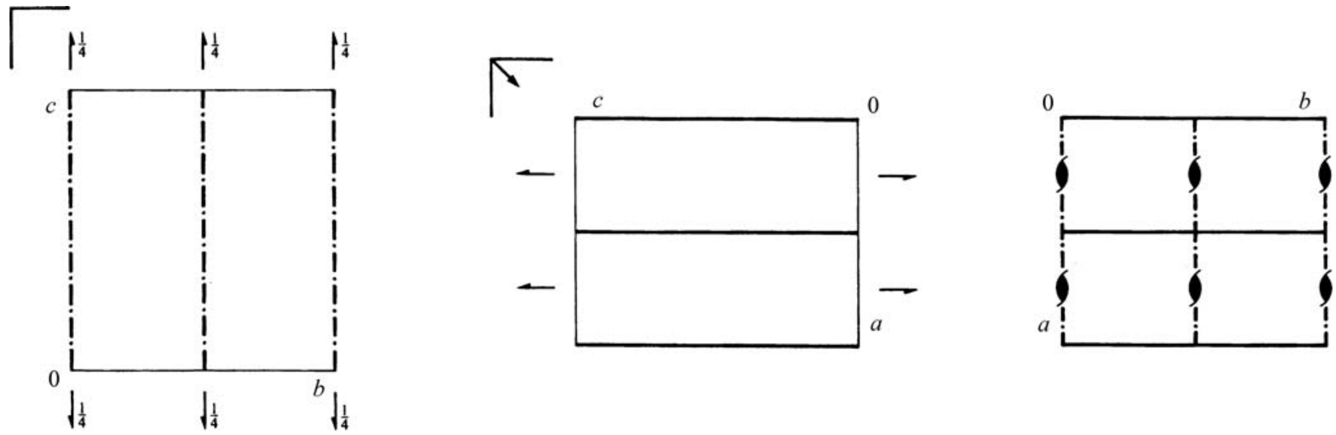

Figure 1.4.5.2
Symmetry-element diagrams for the space group $Pmn2_1$ (31) for orthogonal projections along [100] (left), [010] (middle) and [001] (right).

d *along* [100]: A point x, y, z in a plane perpendicular to the coordinate axis along [100] is mapped to a point x', y', z' in the same plane if $x' = x$, *i.e.* if $x' - x = 0$.

A general operation from the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ maps a point with coordinates x, y, z to a point with coordinates $x' = \bar{x} + \frac{1}{2} + u_1$, $y' = \bar{y} + u_2$, $z' = z + \frac{1}{2} + u_3$ for integers u_1, u_2, u_3. One has $x' - x = -2x + \frac{1}{2} + u_1$ which becomes zero for $x = \frac{1}{4}$ (and $u_1 = 0$) and $x = \frac{3}{4}$ (and $u_1 = 1$), thus operations from the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ fix planes at heights $s = \frac{1}{4}$ and $\frac{3}{4}$. In the left-hand diagram in Fig. 1.4.5.2, the symmetry elements to which these operations belong are indicated by the half-arrows, the label $\frac{1}{4}$ indicating that they are at level $x = \frac{1}{4}$ and $x = \frac{3}{4}$.

An operation from the coset of $\{m_{010}|\frac{1}{2}, 0, \frac{1}{2}\}$ maps x, y, z to $x' = x + \frac{1}{2} + u_1$, $y' = \bar{y} + u_2$, $z' = z + \frac{1}{2} + u_3$ and one has $x' - x = \frac{1}{2} + u_1$. Since this is never zero, no operation from this coset fixes a plane perpendicular to [100].

Finally, an operation from the coset of $\{m_{100}|0\}$ maps x, y, z to $x' = \bar{x} + u_1$, $y' = y + u_2$, $z' = z + u_3$ and one has $x' - x = -2x + u_1$, which becomes zero for $x = 0$ (and $u_1 = 0$) and $x = \frac{1}{2}$ (and $u_1 = 1$). Thus, operations from the coset of $\{m_{100}|0\}$ fix planes at heights $s = 0$ and $\frac{1}{2}$. The symmetry elements of these reflections with mirror plane parallel to the projection plane are indicated by the right-angle symbol in the upper left corner of the left-hand diagram in Fig. 1.4.5.2.

The sectional layer groups are thus layer groups of type $pm11$ (layer group No. 4 with symbol $p11m$ in a non-standard setting) for $s = 0$ and $s = \frac{1}{2}$, of type $p112_1$ (layer group No. 9 with symbol $p2_111$ in a non-standard setting) for $s = \frac{1}{4}$ and $s = \frac{3}{4}$ and of type $p1$ (layer group No. 1) for all other s between 0 and 1. The side-preserving operations are in all cases just the translations.

It is worthwhile noting that in many cases most of the information about the sectional layer groups can be read off the space-group diagrams. In the present example, the left-hand diagram in Fig. 1.4.5.2 displays the twofold screw rotation at height $s = \frac{1}{4}$ (and thus also at $s = \frac{3}{4}$) and the reflection at height $s = 0$ (and thus also at $s = \frac{1}{2}$). On the other hand, the n glide, indicated by the dashed-dotted lines in the diagram, does not give rise to an element of the sectional layer group, because its glide vector has a component along the [100] direction and can thus not fix any layer along this direction.

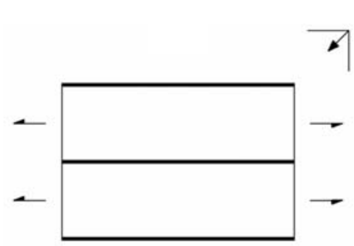

Figure 1.4.5.3
Symmetry-element diagram for the layer group $pm2_1n$ (32).

d *along* [010]: A point x, y, z in a plane perpendicular to the coordinate axis along [010] is mapped to a point x', y', z' in the same plane if $y' = y$, *i.e.* if $y' - y = 0$.

From the calculations above one sees that for operations in the coset of $\{m_{100}|0\}$ one has $y' - y = u_2$, hence operations in this coset fix the plane for any value of s and are side-preserving operations. In the middle diagram in Fig. 1.4.5.2 the symmetry elements for these reflections are indicated by the horizontal solid lines.

For the operations in the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ one has $y' - y = -2y + u_2$, and so these operations fix planes only for $s = 0$ and $s = \frac{1}{2}$. The same is true for the operations in the coset of $\{m_{010}|\frac{1}{2}, 0, \frac{1}{2}\}$, because here one also has $y' - y = -2y + u_2$. The symmetry elements to which the screw rotations belong are indicated by the half arrows in the middle diagram of Fig. 1.4.5.2, and the symmetry elements for the glide reflections are symbolized by the right angle with diagonal arrow in the upper left corner, indicating that the geometric element is a diagonal glide plane.

The sectional layer groups are thus of type $pmn2_1$ (layer group No. 32 with symbol $pm2_1n$ in a non-standard setting) for $s = 0, \frac{1}{2}$ and of type $pm11$ (layer group No. 11) for all other s. The group of side-preserving operations is in all cases of type $pm11$.

In Fig. 1.4.5.3 the diagram of the symmetry elements for the layer group $pm2_1n$ (layer group No. 32) is displayed. It coincides with the middle diagram in Fig. 1.4.5.2 (up to the placement of the symbol for the diagonal glide plane), showing that in this case the sectional layer groups can also be read off directly from the space-group diagrams.

d *along* [001]: A point x, y, z in a plane perpendicular to the coordinate axis along [001] is mapped to a point x', y', z' in the same plane if $z' = z$, *i.e.* if $z' - z = 0$.

As in the case of **d** along [010], operations in the coset of $\{m_{100}|0\}$ fix such a plane for any value of s, since $z' - z = u_3$.

Again, these are side-preserving operations. The symmetry elements to which these reflections belong are indicated by the horizontal solid lines in the right-hand diagram in Fig. 1.4.5.2. For the operations in the cosets of $\{2_{001}|\frac{1}{2},0,\frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2},0,\frac{1}{2}\}$ one has $z'-z=\frac{1}{2}+u_3$, which is never zero (for an integer u_3), and so operations in these cosets never fix a plane perpendicular to [001].

Thus, for any value of s the sectional layer group is of type $pm11$ (layer group No. 11) and contains only side-preserving operations.

1.4.5.3. Projections

As we have seen, a section of a crystal pattern is determined by a vector **d** and a height s along this vector. Choosing two vectors $\mathbf{a}'$ and $\mathbf{b}'$ perpendicular to **d**, the points of the section plane at height s are precisely given by the vectors $x\mathbf{a}'+y\mathbf{b}'+s\mathbf{d}$. In contrast to that, a *projection* of a crystal pattern along **d** is obtained by mapping an arbitrary point $x\mathbf{a}'+y\mathbf{b}'+z\mathbf{d}$ to the point $x\mathbf{a}'+y\mathbf{b}'$ of the plane spanned by $\mathbf{a}'$ and $\mathbf{b}'$, thereby ignoring the coordinate along the **d** direction.

Definition

In a *projection* of a crystal pattern along the *projection direction* **d**, a point X of the crystal pattern is mapped to the intersection of the line through X along **d** with a fixed plane perpendicular to **d**.

One may think of the projection plane as the plane perpendicular to **d** and containing the origin, but every plane perpendicular to **d** will give the same result.

Let L be the line along **d**. If a symmetry operation g of a space group $\mathcal{G}$ maps L to a line parallel to L, then g maps every plane perpendicular to **d** again to a plane perpendicular to **d**. This means that points that are projected to a single point (*i.e.* points on a line parallel to L) are mapped by g to points that are again projected to a single point and thus the operation g gives rise to a symmetry of the projection of the crystal pattern. Conversely, an operation g that maps L to a line that is inclined to L does not result in a symmetry of the projection, since the points on L are projected to a single point, whereas the image points under g are projected to a line. In summary, the operations of $\mathcal{G}$ that map L to a line parallel to L give rise to symmetries of the projection forming a *plane group*, sometimes called a wallpaper group.

Let $\mathcal{H}$ be the subgroup of $\mathcal{G}$ consisting of those $g\in\mathcal{G}$ mapping the line L to a line parallel to L, then $\mathcal{H}$ is called the *scanning group along* **d**. The scanning group $\mathcal{H}$ can be read off a coset decomposition $\mathcal{G}=g_1\mathcal{T}\cup\cdots\cup g_s\mathcal{T}$ relative to the translation subgroup $\mathcal{T}$ of $\mathcal{G}$. Since translations map lines to parallel lines, one only has to check whether a coset representative g_i maps L to a line parallel to L. This is precisely the case if the linear part of g_i maps **d** to **d** or to −**d**. Therefore, $\mathcal{H}$ is the union of those cosets $g_i\mathcal{T}$ relative to $\mathcal{T}$ for which the linear part of g_i maps **d** to **d** or to −**d**.

If the operations of a space group $\mathcal{G}$ are written as augmented matrices with respect to a (usually non-conventional) basis $\mathbf{a}'$, $\mathbf{b}'$, **d** such that $\mathbf{a}'$ and $\mathbf{b}'$ are perpendicular to **d**, then an operation g of the scanning group $\mathcal{H}$ is of the form

$$g=\left(\begin{array}{ccc|c} r_{11} & r_{12} & 0 & t_1\\ r_{21} & r_{22} & 0 & t_2\\ 0 & 0 & r_{33} & t_3\\ \hline 0 & 0 & 0 & 1\end{array}\right)$$

with $r_{33}=\pm1$ (just as for planar sections). Then the action of g on the projection along **d** is obtained by ignoring the z coordinate, *i.e.* by cutting out the upper 2×2 block of the linear part and the first two components of the translation part. This gives rise to the plane-group operation

$$g'=\left(\begin{array}{cc|c} r_{11} & r_{12} & t_1\\ r_{21} & r_{22} & t_2\\ \hline 0 & 0 & 1\end{array}\right).$$

The mapping that assigns to each operation g of the scanning group its action g' on the projection is in fact a homomorphism from $\mathcal{H}$ to a plane group and the kernel $\mathcal{K}$ of this homomorphism are the operations of the form

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & r_{33} & t_3\\ \hline 0 & 0 & 0 & 1\end{array}\right),$$

i.e. translations along **d** and reflections with normal vector parallel to **d**.

Definition

The symmetry group of the projection along the projection direction **d** is the plane group of actions on the projection of those operations of $\mathcal{G}$ that map the line L along **d** to a line parallel to L.

This group is isomorphic to the quotient group of the scanning group $\mathcal{H}$ along **d** by the group $\mathcal{K}$ of translations along **d** and reflections with normal vector parallel to **d**.

Example

We consider again the space group $\mathcal{G}$ of type $Pmn2_1$ (31) for which the augmented matrices of the coset representatives with respect to the translation subgroup (in the standard setting) are given by

$$\{1|0\}=\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ \hline 0 & 0 & 0 & 1\end{array}\right),$$

$$\{2_{001}|\tfrac{1}{2},0,\tfrac{1}{2}\}=\left(\begin{array}{ccc|c} -1 & 0 & 0 & \frac{1}{2}\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & \frac{1}{2}\\ \hline 0 & 0 & 0 & 1\end{array}\right)$$

$$\{m_{010}|\tfrac{1}{2},0,\tfrac{1}{2}\}=\left(\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2}\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & \frac{1}{2}\\ \hline 0 & 0 & 0 & 1\end{array}\right),$$

$$\{m_{100}|0\}=\left(\begin{array}{ccc|c} -1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ \hline 0 & 0 & 0 & 1\end{array}\right).$$

Since the linear parts of all four matrices are diagonal matrices, the scanning group for projections along the coordinate axes is always the full group $\mathcal{G}$.

For the projection along the direction [100], one has to cut out the lower 2×2 part of the linear parts and the second and third component of the translation part, thus choosing $\mathbf{a}' = \mathbf{b}, \mathbf{b}' = \mathbf{c}$ as a basis for the projection plane. This gives as matrices for the projected operations

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

in which the third and fourth operations are clearly redundant and which is thus a plane group of type $p1g1$ (plane group No. 4 with short symbol pg).

The projection along the direction [010] gives for the basis $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{c}$ of the projection plane (thus picking out the first and third rows and columns) the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where the second matrix is the product of the third and fourth. The third operation is a centring translation, the fourth a reflection, thus the resulting plane group is of type $c1m1$ (plane group No. 5 with short symbol cm).

Finally, the projection along the direction [001] results for the basis $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{b}$ of the projection plane in the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where again the second matrix is the product of two others. The third operation is a glide reflection and the fourth is a reflection, thus the corresponding plane group is of type $p2mg$ (plane group No. 7). Note that in order to obtain the plane group $p2mg$ in its standard setting, the origin has to be shifted to $\frac{1}{4}, 0$ (with respect to the plane basis $\mathbf{a}', \mathbf{b}'$).

As for the sectional layer groups, the typical projection directions considered are symmetry directions of the space group $\mathcal{G}$, *i.e.* directions along rotation or screw axes or normal to reflection or glide planes. In order to relate the coordinate system of the plane group to that of the space group, not only the basis vectors $\mathbf{a}', \mathbf{b}'$ perpendicular to the projection direction $\mathbf{d}$ have to be given, but also the origin for the plane group. This is done by specifying a line parallel to the projection direction which is projected to the origin of the plane group in its conventional setting. The space-group tables list the plane groups for the projections along symmetry directions of the group in the block 'Symmetry of special projections'.

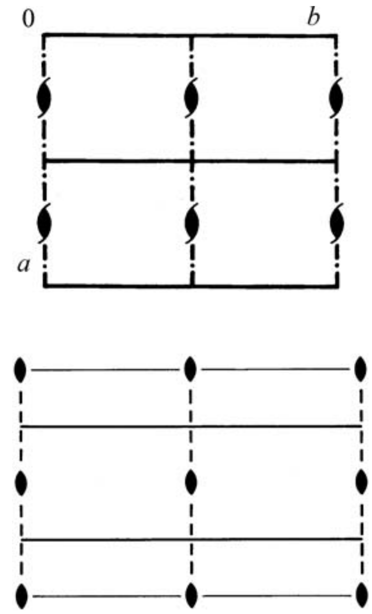

Figure 1.4.5.4
Orthogonal projection along [001] of the symmetry-element diagram for $Pmn2_1$ (31) (top) and the diagram for plane group $p2mg$ (7) (bottom).

It is not hard to determine the corresponding types of plane-group operations for the different types of space-group operations, as is shown by the following list of simple rules:

(i) a translation becomes a translation (possibly the identity);
(ii) an inversion becomes a twofold rotation;
(iii) a k-fold rotation or screw rotation with axis parallel to $\mathbf{d}$ becomes a k-fold rotation;
(iv) a three-, four- or sixfold rotoinversion with axis parallel to $\mathbf{d}$ becomes a six-, four- or threefold rotation, respectively;
(v) a reflection or glide reflection with normal vector parallel to $\mathbf{d}$ becomes a translation (possibly the identity);
(vi) a twofold rotation and a screw rotation with axis perpendicular to $\mathbf{d}$ become a reflection and glide reflection, respectively;
(vii) a reflection or a glide reflection with normal vector perpendicular to $\mathbf{d}$ becomes a reflection or glide reflection depending on whether there is a glide component perpendicular to $\mathbf{d}$ or not.

The relationship between the symmetry operations in three-dimensional space and the corresponding symmetry operations of a projection as listed above can be seen directly in the diagrams of the corresponding groups. In Fig. 1.4.5.4, the top diagram shows the orthogonal projection of the symmetry-element diagram of $Pmn2_1$ along the [001] direction and the bottom diagram shows the diagram for the plane group $p2mg$, which is precisely the symmetry group of the projection of $Pmn2_1$ along [001]. Firstly, one sees immediately that in order to match the two diagrams, the origin in the projection plane has to be shifted to $\frac{1}{4}, 0$ (as already noted in the example above). Secondly, keeping in mind that the projection direction $\mathbf{d}$ is perpendicular to the drawing plane, one sees the correspondence between the twofold screw rotations in $Pmn2_1$ with the twofold rotations in $p2mg$ [rule (iii)], the correspondence between the reflections with normal vector perpendicular to **d** in $Pmn2_1$ and the reflections in $p2mg$ [rule (vii)] and the correspondence between the diagonal glide reflections in $Pmn2_1$ (indicated by the dot-dash lines) and the glide reflections in $p2mg$ {rule (vii); note that the diagonal glide vector has a component perpendicular to the projection direction [001]}.

Example

Let $\mathcal{G}$ be a space group of type $P\bar{4}b2$ (117), then the interesting projection directions (*i.e.* symmetry directions) are [100], [010], [001], [110] and [$\bar{1}$10]. However, the directions [100] and [010] are symmetry-related by the fourfold rotoinversion and thus result in the same projection. The same holds for the directions [110] and [$\bar{1}$10]. The three remaining directions are genuinely different and the projections along these directions will be discussed in detail below. The corresponding information given in the space-group tables under the heading 'Symmetry of special projections' is reproduced in Fig. 1.4.5.5 for $P\bar{4}b2$.

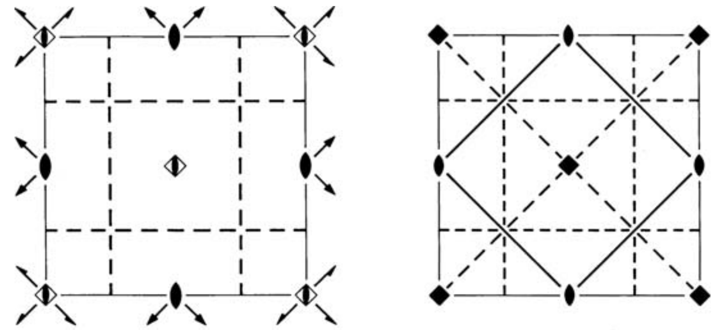

Figure 1.4.5.6
Orthogonal projection along [001] of the symmetry-element diagram for $P\bar{4}b2$ (117) (left) and the diagram for plane group $p4gm$ (12) (right).

Symmetry of special projections

Along [001] $p4gm$	Along [100] $p1m1$	Along [110] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\quad \mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\quad \mathbf{b}' = \mathbf{c}$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $0, 0, z$	Origin at $x, 0, 0$	Origin at $x, x, 0$

Figure 1.4.5.5
'Symmetry of special projections' block of $P\bar{4}b2$ (117) as given in the space-group tables.

Coset representatives of $\mathcal{G}$ relative to its translation subgroup can be extracted from the general-positions block in the space-group tables of $P\bar{4}b2$ and are given in Table 1.4.5.2.

d *along* [001]: The linear parts of all coset representatives map [001] to $\pm$[001], and therefore the scanning group $\mathcal{H}$ is the full group $\mathcal{G}$. A conventional basis for the translations of the projection is $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$. The operation g_3 acts as a fourfold rotation, g_5 acts as a glide reflection with normal vector $\mathbf{b}'$ and g_8 as a reflection with normal vector $\mathbf{a}' + \mathbf{b}'$. Thus, the resulting plane group has type $p4gm$ (plane group No. 12). The line parallel to the projection direction [001] which is projected to the origin of $p4gm$ in its conventional setting is the line 0, 0, z.

Again, it is instructive to look at the symmetry-element diagrams for the respective space and plane groups, as displayed in Fig. 1.4.5.6. The twofold rotations and fourfold rotoinversions with axis along [001] are turned into twofold rotations and fourfold rotations, respectively [rules (iii) and (iv)]. The glide reflections with both normal vector and glide vector perpendicular to [001] (dashed lines) result in glide reflections [rule (vii)]. The twofold rotations (full arrows) and screw rotations (half arrows) with rotation axis perpendicular to [001] give reflections and glide reflections, respectively [rule (vi)]. Note that the two diagrams can be matched directly, because the line 0, 0, z which is projected to the origin of $p4gm$ runs through the origin of $P\bar{4}b2$.

Table 1.4.5.2
Coset representatives of $P\bar{4}b2$ (117) relative to its translation subgroup

	Coordinate triplet	Description
g_1:	x, y, z	Identity
g_2:	$\bar{x}, \bar{y}, z$	Twofold rotation with axis along [001]
g_3:	$y, \bar{x}, \bar{z}$	Fourfold rotoinversion with axis along [001]
g_4:	$\bar{y}, x, \bar{z}$	Fourfold rotoinversion with axis along [001]
g_5:	$x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$	Glide reflection with normal vector [010] and glide component along [100]
g_6:	$\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$	Glide reflection with normal vector [100] and glide component along [010]
g_7:	$y + \frac{1}{2}, x + \frac{1}{2}, \bar{z}$	Twofold screw rotation with axis parallel to [110]
g_8:	$\bar{y} + \frac{1}{2}, \bar{x} + \frac{1}{2}, \bar{z}$	Twofold rotation with axis parallel to [1$\bar{1}$0]

d *along* [100]: Only the linear parts of the coset representatives g_1, g_2, g_5 and g_6 map [100] to $\pm$[100], thus these four cosets form the scanning group $\mathcal{H}$ (which is of index 2 in $\mathcal{G}$). The operation g_6 acts as a translation by $\frac{1}{2}\mathbf{b}$, thus a conventional basis for the translations of the projection is $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ and $\mathbf{b}' = \mathbf{c}$. The operation g_2 acts as a reflection with normal vector $\mathbf{a}'$ and g_5 acts as the same reflection composed with the translation $\mathbf{a}'$. The resulting plane group is thus of type $p1m1$ (plane group No. 3 with short symbol pm). The line which is mapped to the origin of $p1m1$ in its conventional setting is x, 0, 0.

d *along* [110]: Only the linear parts of the coset representatives g_1, g_2, g_7 and g_8 map [110] to $\pm$[110], thus these four cosets form the scanning group $\mathcal{H}$ (of index 2 in $\mathcal{G}$). The translation by **b** is projected to a translation by $\frac{1}{2}(-\mathbf{a} + \mathbf{b})$, thus a conventional basis for the translations of the projection is $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ and $\mathbf{b}' = \mathbf{c}$. The operation g_2 acts as a reflection with normal vector $\mathbf{a}'$, g_7 acts as a twofold rotation and g_8 acts as a reflection with normal vector $\mathbf{b}'$. The resulting plane group is thus of type $p2mm$ (plane group No. 6). The line parallel to the projection direction [110] that is mapped to the origin of $p2mm$ (in its conventional setting) is x, x, 0.

Note that for directions different from those considered above, additional non-trivial plane groups may be obtained. For example, for the projection direction $\mathbf{d} = [1\bar{1}1]$, the scanning group consists of the cosets of g_1 and g_7. The operation g_7 acts as a glide reflection and the resulting plane group is of type $c1m1$ (plane group No. 5).

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