International Tables for Crystallography (2016). Vol. A, Section 1.4.2, pp. 50–59.

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	$z, \bar{x}, y$	$\bar{3}^{+}$	$\bar{x}, \bar{x}, x$	$3^{+}_{\bar{1}\bar{1}1}$
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 *p*4*mm*, while those of Table 1.4.2.5 correspond to the general-position sequence of the plane group *p*6*mm*. 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 *Fmm*2 (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 *Fmm*2 (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

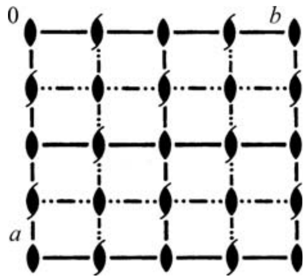

Figure 1.4.2.3
Symmetry-element diagram for space group *Fmm*2 (42) (orthogonal projection along [001]).

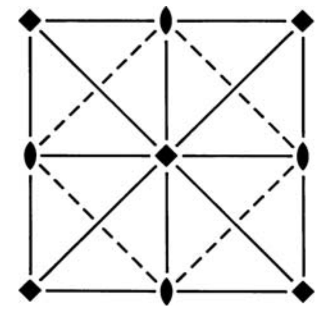

Figure 1.4.2.5
Symmetry-element diagram for space group *P*4*mm* (99) (orthogonal projection along [001]).

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].

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).

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.

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.

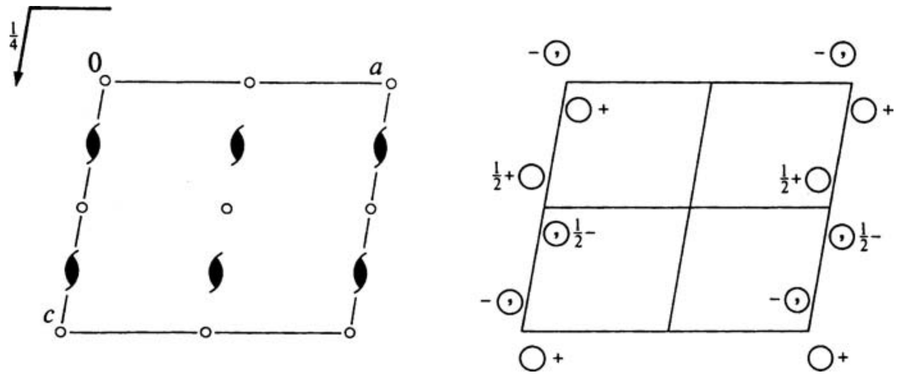

Figure 1.4.2.6
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2_1/c$, No. 14 (unique axis b, cell choice 1).

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

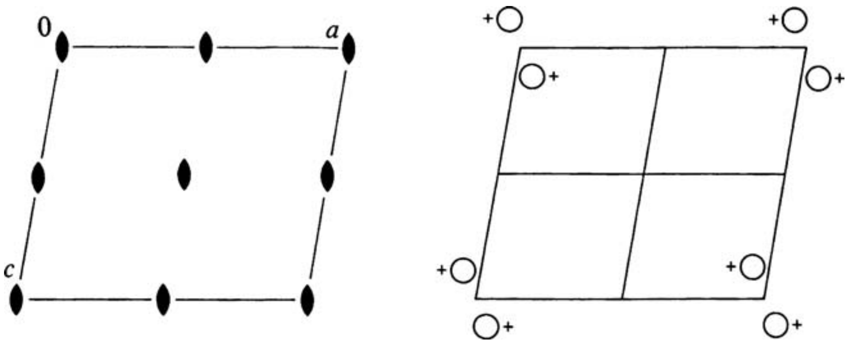

Figure 1.4.2.7
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2$, No. 3 (unique axis b, cell choice 1).

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

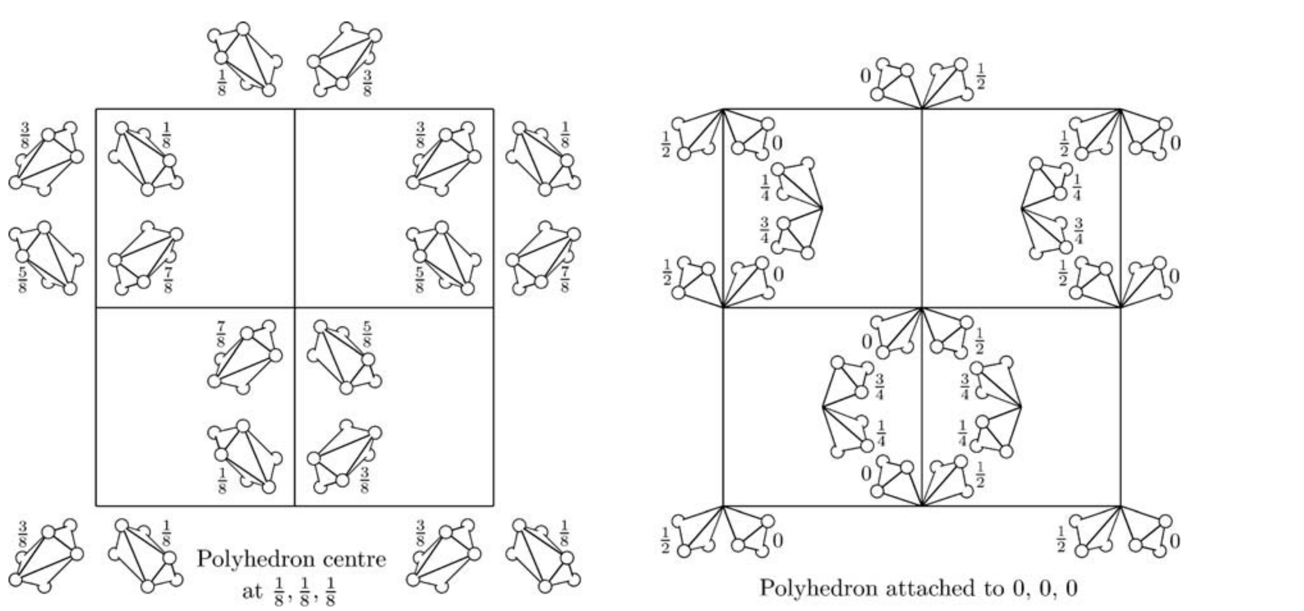

Figure 1.4.2.8
General-position diagrams for the space group $I4_132$ (214). Left: polyhedra (twisted trigonal antiprisms) with centres at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points (site-symmetry group .32). Right: polyhedra (sphenoids) attached to 0, 0, 0 and its equivalent points (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 *P*2, 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 *P*2/*m* type, and not of *P*2. There are a number of space groups for which the general-position diagram displays higher space-group symmetry, for example: *P*1, $P2_1$, *P*4*mm*, *P*6 *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	$2_{001}, 2_{010}$
*mm*2	$2_{001}, m_{010}$
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	$2_{001}, 4^+_{001}, 2_{010}$
4*mm*	$2_{001}, 4^+_{001}, m_{010}$
$\bar{4}2m$	$2_{001}, \bar{4}^+_{001}, 2_{010}$
$\bar{4}m2$	$2_{001}, \bar{4}^+_{001}, m_{010}$
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	$3^+_{001}, 2_{1\bar{1}0}$
3*m*1	$3^+_{001}, m_{110}$
(rhombohedral coordinates	$3^+_{111}, m_{\bar{1}01}$)
31*m*	$3^+_{001}, m_{1\bar{1}0}$
$\bar{3}m1$	$3^+_{001}, 2_{110}, \bar{1}$
(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	$3^+_{001}, 2_{001}, 2_{110}$
6*mm*	$3^+_{001}, 2_{001}, m_{110}$
$\bar{6}m2$	$3^+_{001}, m_{001}, m_{110}$
$\bar{6}2m$	$3^+_{001}, m_{001}, 2_{110}$
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

references