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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

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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

references