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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.

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

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 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 $\frac{1}{3}\mathbf{c}$.

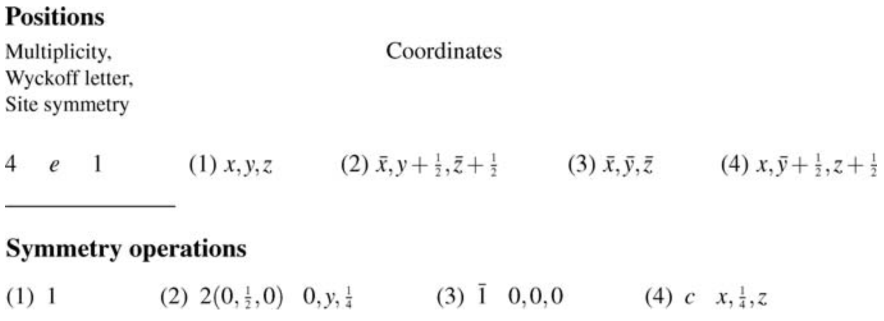
A *reflection* is symbolized by the letter m, followed by the location of the mirror plane.

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.

references