International Tables for Crystallography (2006). Vol. A, Section 4.3.5, pp. 73–75.

Examples

(1) $P4_2/mbc$ (135). From the full symbol, the *first* maximal t subgroup is found to be $P2_1/b\,2_1/a\,2/m$ ($Pbam$). The C-cell symbol is $C4_2/m\,cg_1$ and gives rise to the *second* maximal orthorhombic t subgroup $Cccm$, cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

(2) $I4/m\,cm$ (140). Similarly, the *first* orthorhombic maximal t subgroup is $Iccm$ ($Ibam$); the *second* maximal orthorhombic t subgroup is obtained from the F-cell symbol as $F\overset{ban}{c}\,c\,\underset{mmn}{m}$ ($Fmmm$), cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

These examples show that P- and C-cell, as well as I- and F-cell descriptions of tetragonal groups have to be considered together.

(iii) *Monoclinic subgroups*

Only space groups of classes 4, $\bar{4}$ and $4/m$ have maximal monoclinic t subgroups.

Examples

(1) $P4_1$ (76) has the subgroup $P112_1$ ($P2_1$). The C-cell description does not add new features: $C112_1$ is reducible to $P2_1$.

(2) $I4_1/a$ (88) has the subgroup $I112_1/a$, equivalent to $I112/a$ ($C2/c$). The F-cell description yields the same subgroup $F11\,2/d$, again reducible to $C2/c$.

4.3.5. Trigonal and hexagonal systems

The trigonal and hexagonal crystal systems are considered together, because they form the hexagonal 'crystal family', as explained in Chapter 2.1. Hexagonal lattices occur in both systems, whereas rhombohedral lattices occur only in the trigonal system.

4.3.5.1. *Historical note*

The 1935 edition of *International Tables* contains the symbols C and H for the *hexagonal lattice* and R for the *rhombohedral lattice.* C recalls that the hexagonal lattice can be described by a double rectangular C-centred cell (orthohexagonal axes); H was used for a hexagonal triple cell (see below); R designates the rhombohedral lattice and is used for both the rhombohedral description (primitive cell) and the hexagonal description (triple cell).

In the 1952 edition the following changes took place (*cf.* pages x, 51 and 544 of *IT* 1952): The lattice symbol C was replaced by P for reasons of consistency; the H description was dropped. The symbol R was kept for both descriptions, rhombohedral and hexagonal. The tertiary symmetry element in the short Hermann–Mauguin symbols of class 622, which was omitted in *IT* (1935), was re-established.

In the present volume, the use of P and R is the same as in *IT* (1952). The H cell, however, reappears in the sub- and supergroup data of Part 7 and in Table 4.3.2.1 of this section, where short symbols for the H description of trigonal and hexagonal space groups are given. The C cell reappears in the subgroup data for all trigonal and hexagonal space groups having symmetry elements orthogonal to the main axis.

4.3.5.2. *Primitive cells*

The primitive cells of the hexagonal and the rhombohedral lattice, hP and hR, are defined in Table 2.1.2.1 In Part 7, the 'rhombohedral' description of the hR lattice is designated by 'rhombohedral axes'; *cf.* Chapter 1.2.

4.3.5.3. *Multiple cells*

Multiple cells are frequently used to describe both the hexagonal and the rhombohedral lattice.

(i) *The triple hexagonal R cell; cf. Chapters 1.2 and 2.1*

When the lattice is *rhombohedral hR* (primitive cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$), the triple R cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ corresponds to the 'hexagonal description' of the rhombohedral lattice. There are three right-handed *obverse R* cells:

$$\begin{aligned}
R_1: &\quad \mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{b} - \mathbf{c}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c};\\
R_2: &\quad \mathbf{a}' = \mathbf{b} - \mathbf{c}; \quad \mathbf{b}' = \mathbf{c} - \mathbf{a}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c};\\
R_3: &\quad \mathbf{a}' = \mathbf{c} - \mathbf{a}; \quad \mathbf{b}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}.
\end{aligned}$$

Three further right-handed R cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a 180° rotation around $\mathbf{c}'$. These cells are *reverse*. The transformations between the triple R cells and the primitive rhombohedral cell are given in Table 5.1.3.1 and Fig. 5.1.3.6.

The obverse triple R cell has 'centring points' at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3},$$

whereas the reverse R cell has 'centring points' at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{2}{3}.$$

In the space-group tables of Part 7, the obverse R_1 cell is used, as illustrated in Fig. 2.2.6.9. This 'hexagonal description' is designated by 'hexagonal axes'.

(ii) *The triple rhombohedral D cell*

Parallel to the 'hexagonal description of the rhombohedral lattice' there exists a 'rhombohedral description of the hexagonal lattice'. Six right-handed rhombohedral cells (here denoted by D) with cell vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of equal lengths are obtained from the hexagonal P cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ by the following transformations and by cyclic permutations of $\mathbf{a}', \mathbf{b}', \mathbf{c}'$:

$$\begin{aligned}
D_1: &\quad \mathbf{a}' = \mathbf{a} + \mathbf{c}; \quad \mathbf{b}' = \mathbf{b} + \mathbf{c}; \quad \mathbf{c}' = -(\mathbf{a} + \mathbf{b}) + \mathbf{c}\\
D_2: &\quad \mathbf{a}' = -\mathbf{a} + \mathbf{c}; \quad \mathbf{b}' = -\mathbf{b} + \mathbf{c}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}.
\end{aligned}$$

The transformation matrices are listed in Table 5.1.3.1. D_2 follows from D_1 by a 180° rotation around [111]. The D cells are triple rhombohedral cells with 'centring' points at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{2}{3},\tfrac{2}{3}.$$

The D cell, not used in practice and not considered explicitly in the present volume, is useful for a deeper understanding of the relations between hexagonal and rhombohedral lattices.

(iii) *The triple hexagonal H cell; cf. Chapter 1.2*

Generally, a hexagonal lattice hP is described by means of the smallest hexagonal P cell. An alternative description employs a larger hexagonal H-centred cell of three times the volume of the P cell; this cell was extensively used in *IT* (1935), see *Historical note* above.

There are three right-handed orientations of the H cell (basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$) with respect to the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the P cell:

$$\begin{aligned}
H_1: &\quad \mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{a} + 2\mathbf{b}; \quad \mathbf{c}' = \mathbf{c}\\
H_2: &\quad \mathbf{a}' = 2\mathbf{a} + \mathbf{b}; \quad \mathbf{b}' = -\mathbf{a} + \mathbf{b}; \quad \mathbf{c}' = \mathbf{c}\\
H_3: &\quad \mathbf{a}' = \mathbf{a} + 2\mathbf{b}; \quad \mathbf{b}' = -2\mathbf{a} - \mathbf{b}; \quad \mathbf{c}' = \mathbf{c}.
\end{aligned}$$

The transformations are given in Table 5.1.3.1 and Fig. 5.1.3.8. The new vectors $\mathbf{a}'$ and $\mathbf{b}'$ are rotated in the ab plane by $-30°(H_1)$, $+30°(H_2)$, $+90°(H_3)$ with respect to the old vectors $\mathbf{a}$ and $\mathbf{b}$. Three further right-handed H cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a rotation of 180° around $\mathbf{c}'$.

The H cell has 'centring' points at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},0; \quad \tfrac{1}{3},\tfrac{2}{3},0.$$

Secondary and tertiary symmetry elements of the P cell are interchanged in the H cell, and the general position in the H cell is easily obtained, as illustrated by the following example.

Example

The space-group symbol $P3m1$ in the P cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ becomes $H31m$ in the H cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. To obtain the general position of $H31m$, consider the coordinate triplets of $P31m$ and add the centring translations $0, 0, 0$; $\frac{2}{3}, \frac{1}{3}, 0$; $\frac{1}{3}, \frac{2}{3}, 0$.

(iv) *The double orthohexagonal C cell*

The C-centred cell which is defined by the so-called 'orthohexagonal' vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ has twice the volume of the P cell. There are six right-handed orientations of the C cell, which are C_1, C_2 and C_3 plus three further ones obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$:

$$\begin{aligned}
C_1 &: \mathbf{a}' = \mathbf{a}\phantom{{}+\mathbf{b}}; & \mathbf{b}' &= \mathbf{a} + 2\mathbf{b}; & \mathbf{c}' &= \mathbf{c}\\
C_2 &: \mathbf{a}' = \mathbf{a} + \mathbf{b}; & \mathbf{b}' &= -\mathbf{a} + \mathbf{b}; & \mathbf{c}' &= \mathbf{c}\\
C_3 &: \mathbf{a}' = \phantom{\mathbf{a}+{}}\mathbf{b}; & \mathbf{b}' &= -2\mathbf{a} - \mathbf{b}; & \mathbf{c}' &= \mathbf{c}.
\end{aligned}$$

Transformation matrices are given in Table 5.1.3.1 and illustrations in Fig. 5.1.3.7. Here $\mathbf{b}'$ is the long axis.

4.3.5.4. *Relations between symmetry elements*

In the hexagonal crystal classes $62(2)$, $6m(m)$ and $\bar{6}2(m)$ or $\bar{6}m(2)$, where the tertiary symmetry element is between parentheses, the following products hold:

$$6 \times 2 = (2) = \bar{6} \times m; \quad 6 \times m = (m) = \bar{6} \times 2$$

or

$$6 \times 2 \times (2) = 6 \times m \times (m) = \bar{6} \times 2 \times (m) = \bar{6} \times m \times (2) = 1.$$

The same relations hold for the corresponding Hermann–Mauguin space-group symbols.

4.3.5.5. *Additional symmetry elements*

Parallel axes 2 and 2_1 occur perpendicular to the principal symmetry axis. Examples are space groups $R32$ (155), $P321$ (150) and $P312$ (149), where the screw components are $\frac{1}{2}, \frac{1}{2}, 0$ (rhombohedral axes) or $\frac{1}{2}, 0, 0$ (hexagonal axes) for $R32$; $\frac{1}{2}, 0, 0$ for $P321$; and $\frac{1}{2}, 1, 0$ for $P312$. Hexagonal examples are $P622$ (177) and $P\bar{6}2c$ (190).

Likewise, mirror planes m parallel to the main symmetry axis alternate with glide planes, the glide components being perpendicular to the principal axis. Examples are $P3m1$ (156), $P31m$ (157), $R3m$ (160) and $P6mm$ (183).

Glide planes c parallel to the main axis are interleaved by glide planes n. Examples are $P3c1$ (158), $P31c$ (159), $R3c$ (161, hexagonal axes), $P\bar{6}c2$ (188). In $R3c$ and $R\bar{3}c$, the glide component $0, 0, \frac{1}{2}$ for hexagonal axes becomes $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ for rhombohedral axes, *i.e.* the c glide changes to an n glide. Thus, if the space group is referred to rhombohedral axes, diagonal n planes alternate with diagonal a, b or c planes (*cf.* Section 1.4.4).

In R space groups, all additional symmetry elements with glide and screw components have their origin in the action of an integral lattice translation. This is also true for the axes 3_1 and 3_2 which appear in all R space groups (*cf.* Table 4.1.2.2). For this reason, the 'rhombohedral centring' R is not included in Table 4.1.2.3, which contains only the centrings A, B, C, I, F.

4.3.5.6. *Group–subgroup relations*

4.3.5.6.1. *Maximal k subgroups*

Maximal k subgroups of index [3] are obtained by 'decentring' the triple cells R (hexagonal description), D and H in the trigonal system, H in the hexagonal system. Any one of the three centring points may be taken as origin of the subgroup.

(i) *Trigonal system*

Examples

(1) $P3m1$ (156) (cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) is equivalent to $H31m$ ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}$). Decentring of the H cell yields maximal non-isomorphic k subgroups of type $P31m$. Similarly, $P31m$ (157) has maximal subgroups of type $P3m1$; thus, one can construct infinite chains of subgroup relations of index [3], tripling the cell at each step:

$$P3m1 \rightarrow P31m \rightarrow P3m1 \ldots$$

(2) $R3$ (146), by decentring the triple hexagonal R cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$, yields the subgroups $P3$, $P3_1$ and $P3_2$ of index [3].

(3) Likewise, decentring of the triple rhombohedral cells D_1 and D_2 gives rise, for each cell, to the rhombohedral subgroups of a trigonal P group, again of index [3].

Combining (2) and (3), one may construct infinite chains of subgroup relations, tripling the cell at each step:

$$P3 \rightarrow R3 \rightarrow P3 \rightarrow R3 \ldots$$

These chains illustrate best the connections between rhombohedral and hexagonal lattices.

(4) Special care must be applied when secondary or tertiary symmetry elements are present. Combining (1), (2) and (3), one has for instance:

$$P31c \rightarrow R3c \rightarrow P3c1 \rightarrow P31c \rightarrow R3c \ldots$$

(5) Rhombohedral subgroups, found by decentring the triple cells D_1 and D_2, are given under block **IIb** and are referred there to hexagonal axes, $\mathbf{a}', \mathbf{b}', \mathbf{c}$ as listed below. Examples are space groups $P3$ (143) and $P\bar{3}1c$ (163)

$$\begin{aligned}
\mathbf{a}' &= \mathbf{a} - \mathbf{b}, & \mathbf{b}' &= \mathbf{a} + 2\mathbf{b}, & \mathbf{c}' &= 3\mathbf{c};\\
\mathbf{a}' &= 2\mathbf{a} + \mathbf{b}, & \mathbf{b}' &= -\mathbf{a} + \mathbf{b}, & \mathbf{c}' &= 3\mathbf{c}.
\end{aligned}$$

(ii) *Hexagonal system*

Examples

(1) $P\bar{6}2c$ (190) is described as $H\bar{6}c2$ in the triple cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$; decentring yields the non-isomorphic subgroup $P\bar{6}c2$.

(2) $P6/mcc$ (192) (cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$) keeps the same symbol in the H cell and, consequently, gives rise to the maximal isomorphic subgroup $P6/mcc$ with cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. An analogous result applies whenever secondary and tertiary symmetry elements in the Hermann–Mauguin symbol are the same and also to space groups of classes 6, $\bar{6}$ and $6/m$.

4.3.5.6.2. *Maximal t subgroups*

Maximal t subgroups of index [2] are read directly from the full symbol of the space groups of classes 32, $3m$, $\bar{3}m$, 622, $6mm$, $\bar{6}2m$, $6/mmm$.

Maximal t subgroups of index [3] follow from the third power of the main-axis operation. Here the C-cell description is valuable.

(i) *Trigonal system*

(*a*) *Trigonal subgroups*

Examples

(1) $R\bar{3}2/c$ (167) has $R3c$, $R32$ and $R\bar{3}$ as maximal t subgroups of index [2].

(2) $P\bar{3}c1$ (165) has $P3c1$, $P321$ and $P\bar{3}$ as maximal t subgroups of index [2].

(*b*) *Orthorhombic subgroups*

No orthorhombic subgroups of trigonal space groups exist, in spite of the existence of an orthohexagonal C cell.

(*c*) *Monoclinic subgroups*

All trigonal space groups with secondary or tertiary symmetry elements have monoclinic C-centred maximal t subgroups of index [3].

Example

$P\bar{3}1c$ (163), $P\bar{3}c1$ (165) and $R\bar{3}c$ (167) have subgroups of type $C2/c$.

(*d*) *Triclinic subgroups*

All trigonal space groups without secondary or tertiary symmetry elements have triclinic maximal t subgroups of index [3].

Example

$P\bar{3}$ (147) and $R\bar{3}$ (148) have subgroups $P\bar{1}$.

(ii) *Hexagonal system*

(*a*) *Hexagonal subgroups*

Example

$P6_3/m\,2/c\,2/m$ (193) has maximal t subgroups $P6_3/m$, $P6_322$, $P6_3cm$, $P\bar{6}2m$ and $P\bar{6}c2$ of index [2].

(*b*) *Trigonal subgroups*

The second and fourth powers of sixfold operations are threefold operations; thus, all hexagonal space groups have maximal trigonal t subgroups of index [2]. In space groups of classes 622, $6mm$, $\bar{6}2m$, $6/mmm$ with secondary and tertiary symmetry elements, trigonal t subgroups always occur in pairs.

Examples

(1) $P6_1$ (169) contains $P3_1$ of index [2].
(2) $P\bar{6}2c$ (190) has maximal t subgroups $P321$ and $P31c$; $P6_122$ (178) has subgroups $P3_121$ and $P3_112$, all of index [2].
(3) $P6_3/mcm$ (193) contains the operation $\bar{3}$ $[= (6_3)^2 \times \bar{1}]$ and thus has maximal t subgroups $P\bar{3}c1$ and $P\bar{3}1m$ of index [2].

(*c*) *Orthorhombic and monoclinic subgroups*

The third power of the sixfold operation is a twofold operation: accordingly, maximal orthorhombic t subgroups of index [3] are derived from the C-cell description of space groups of classes 622, $6mm$, $\bar{6}2m$ and $6/mmm$. Monoclinic P subgroups of index [3] occur in crystal classes 6, $\bar{6}$ and $6/m$.

Examples

(1) $P\bar{6}2c$ (190) becomes $C\bar{6}2c$ in the C cell; with $(\bar{6})^3 = m$, one obtains $C2cm$ (sequence **a**, **b**, **c**) as a maximal t subgroup of index [3]. The standard symbol is $Ama2$.
(2) $P6_3/mcm$ (193) has maximal orthorhombic t subgroups of type $Cmcm$ of index [3]. With the examples under (*a*) and (*b*), this exhausts all maximal t subgroups of $P6_3/mcm$.
(3) $P6_1$ (169) has a maximal t subgroup $P2_1$; $P6_3/m$ (176) has $P2_1/m$ as a maximal t subgroup.

4.3.6. Cubic system

4.3.6.1. *Historical note and arrangement of tables*

In the synoptic tables of *IT* (1935) and *IT* (1952), for cubic space groups short and full Hermann–Mauguin symbols were listed. They agree, except that in *IT* (1935) the tertiary symmetry element of the space groups of class 432 was omitted; it was re-established in *IT* (1952).

In the present edition, the symbols of *IT* (1952) are retained, with one exception. In the space groups of crystal classes $m\bar{3}$ and $m\bar{3}m$, the short symbols contain $\bar{3}$ instead of 3 (*cf.* Section 2.2.4). In Table 4.3.2.1, short and full symbols for all cubic space groups are given. In addition, for centred groups F and I and for P groups with tertiary symmetry elements, extended space-group symbols are listed. In space groups of classes 432 and $\bar{4}3m$, the product rule (as defined below) is applied in the first line of the extended symbol.

4.3.6.2. *Relations between symmetry elements*

Conventionally, the representative directions of the primary, secondary and tertiary symmetry elements are chosen as [001], [111], and $[1\bar{1}0]$ (*cf.* Table 2.2.4.1 for the equivalent directions). As in tetragonal and hexagonal space groups, tertiary symmetry elements are not independent. In classes 432, $\bar{4}3m$ and $m\bar{3}m$, there are product rules

$$4 \times 3 = (2); \quad \bar{4} \times 3 = (m) = 4 \times \bar{3},$$

where the tertiary symmetry element is in parentheses; analogous rules hold for the space groups belonging to these classes. When the symmetry directions of the primary and secondary symmetry elements are chosen along [001] and [111], respectively, the tertiary symmetry direction is [011], according to the product rule. In order to have the tertiary symmetry direction along $[1\bar{1}0]$, one has to choose the somewhat awkward primary and secondary symmetry directions [010] and $[\bar{1}1\bar{1}]$.

Examples

(1) In $P\bar{4}3n$ (218), with the choice of the 3 axis along $[\bar{1}1\bar{1}]$ and of the $\bar{4}$ axis parallel to [010], one finds $\bar{4} \times 3 = n$, the n glide plane being in x, x, z, as shown in the space-group diagram.
(2) In $F\bar{4}3c$ (219), one has the same product rule as above; the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$, however, associates with the n glide plane a c glide plane, also located in x, x, z (*cf.* Table 4.1.2.3). In the space-group diagram and symbol, c was preferred to n.

4.3.6.3. *Additional symmetry elements*

Owing to periodicity, the tertiary symmetry elements alternate; diagonal axes 2 alternate with parallel screw axes 2_1; diagonal planes m alternate with parallel glide planes g; diagonal n planes, *i.e.* planes with glide components $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, alternate with glide planes a, b or c (*cf.* Chapter 4.1 and Tables 4.1.2.2 and 4.1.2.3). For the meaning of the various glide planes g, see Section 11.1.2 and the entries *Symmetry operations* in Part 7.

4.3.6.4. *Group–subgroup relations*

4.3.6.4.1. *Maximal k subgroups*

The extended symbol of $Fm\bar{3}$ (202) shows clearly that $Pm\bar{3}$, $Pn\bar{3}$, $Pb\bar{3}$ ($Pa\bar{3}$) and $Pa\bar{3}$ are maximal subgroups. $Pm\bar{3}m$, $Pn\bar{3}n$, $Pm\bar{3}n$ and $Pn\bar{3}m$ are maximal subgroups of $Im\bar{3}m$ (229). Space groups with d glide planes have no k subgroup of lattice P.

4.3.6.4.2. *Maximal t subgroups*

(*a*) *Cubic subgroups*

The cubic space groups of classes $m\bar{3}$, 432 and $\bar{4}3m$ have maximal cubic subgroups of class 23 which are found by simple inspection of the full symbol.

references