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 **a**, **b**, **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 $-\mathbf{b}'$:

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

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 **a**, **b**, **c**) is equivalent to $H31m$ ($\mathbf{a}'$, $\mathbf{b}'$, **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 **a**, **b**, **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].

references