International Tables for Crystallography (2006). Vol. A, Section 4.3.4, pp. 71–73.

4.3.3.2.2. *Maximal t subgroups of type* **I**

(i) *Orthorhombic subgroups*

The standard full symbol of a P group of class mmm indicates all the symmetry elements, so that maximal t subgroups can be read at once.

Example

$P\,2_1/m2/m2/a$ (51) has the following four t subgroups: $P2_122$ ($P222_1$); $Pmm2$; $P2_1ma$ ($Pmc2_1$); $Pm2a$ ($Pma2$).

From the standard full symbol of an I group of class mmm, the t subgroup of class 222 is read directly. It is either $I222$ [for $Immm$ (71) and $Ibam$ (72)] or $I2_12_12_1$ [for $Ibca$ (73) and $Imma$ (74)]. Use of the two-line symbols results in three maximal t subgroups of class $mm2$.

Example

$Ibam$ (72) has the following three maximal t subgroups of ccn
class $mm2$: $Iba2$; $Ib2_1m$ ($Ima2$); $I2_1am$ ($Ima2$).

From the standard full symbol of a C group of class mmm, one immediately reads the maximal t subgroup of class 222, which is either $C222_1$ [for $Cmcm$ (63) and $Cmce$ (64)] or $C222$ (for all other cases). For the three maximal t subgroups of class $mm2$, the two-line symbols are used.

Example

$Cmce$ (64) has the following three maximal t subgroups of bna
class $mm2$: $Cmc2_1$; $Cm2e$ ($Aem2$); $C2ce$ ($Aea2$).

Finally, $Fmmm$ (69) has maximal t subgroups $F222$ and $Fmm2$ (plus permutations), whereas $Fddd$ (70) has $F222$ and $Fdd2$ (plus permutations).

(ii) *Monoclinic subgroups*

These subgroups are obtained by substituting the symbol '1' in two of the three positions. Non-standard centred cells are reduced to primitive cells.

Examples

(1) $C222_1$ (20) has the maximal t subgroups $C211$ ($C2$), $C121$ ($C2$) and $C112_1$. The last one reduces to $P112_1$ ($P2_1$).
(2) $Ama2$ (40) has the maximal t subgroups $Am11$, reducible to Pm, $A1a1$ (Cc) and $A112$ ($C2$).
(3) $Pnma$ (62) has the standard full symbol $P2_1/n2_1/m2_1/a$, from which the maximal t subgroups $P2_1/n11$ ($P2_1/c$), $P12_1/m1$ ($P2_1/m$) and $P112_1/a$ ($P2_1/c$) are obtained.
(4) $Fddd$ (70) has the maximal t subgroups $F2/d11$, $F12/d1$ and $F112/d$, each one reducible to $C2/c$.

4.3.4. Tetragonal system

4.3.4.1. *Historical note and arrangement of the tables*

In the 1935 edition of *International Tables*, for each tetragonal P and I space group an additional C-cell and F-cell description was given. In the corresponding space-group symbols, secondary and tertiary symmetry elements were simply interchanged. Coordinate triplets for these larger cells were not printed, except for the space groups of class $\bar{4}m2$. In *IT* (1952), the C and F cells were dropped from the space-group tables but kept in the comparative tables.

In the present edition, the C and F cells reappear in the sub- and supergroup tabulations of Part 7, as well as in the synoptic Table 4.3.2.1, where short and extended (two-line) symbols are given for P and C cells, as well as for I and F cells.

4.3.4.2. *Relations between symmetry elements*

In the crystal classes $42(2)$, $4m(m)$, $\bar{4}2(m)$ or $\bar{4}m(2)$, $4/m\,2/m\,(2/m)$, where the tertiary symmetry elements are between parentheses, one finds

$$4\times m=(m)=\bar{4}\times 2;\;\; 4\times 2=(2)=\bar{4}\times m.$$

Analogous relations hold for the space groups. In order to have the symmetry direction of the tertiary symmetry elements along $[1\bar{1}0]$ (*cf.* Table 2.2.4.1), one has to choose the primary and secondary symmetry elements in the product rule along [001] and [010].

Example

In $P4_12(2)$ (91), one has $4_1\times 2=(2)$ so that $P4_12$ would be the short symbol. In fact, in *IT* (1935), the tertiary symmetry element was suppressed for all groups of class 422, but re-established in *IT* (1952), the main reason being the generation of the fourfold rotation as the product of the secondary and tertiary symmetry operations: $4=(m)\times m$ *etc.*

4.3.4.3. *Additional symmetry elements*

As a result of periodicity, in all space groups of classes 422, $\bar{4}m2$ and $4/m\,2/m\,2/m$, the two tertiary diagonal axes 2, along $[1\bar{1}0]$ and [110], alternate with axes 2_1, the screw component being $\frac{1}{2},\mp\frac{1}{2},0$ (*cf.* Table 4.1.2.2).

Likewise, tertiary diagonal mirrors m in x,x,z and $x,\bar{x},z$ in space groups of classes $4mm$, $\bar{4}2m$ and $4/m\,2/m\,2/m$ alternate with glide planes called g,* the glide components being $\frac{1}{2}$, $\pm\frac{1}{2}$, 0. The same glide components produce also an alternation of diagonal glide planes c and n (*cf.* Table 4.1.2.2).

4.3.4.4. *Multiple cells*

The transformations from the P to the two C cells, or from the I to the two F cells, are

$$C_1 \text{ or } F_1\text{: (i)}\quad \mathbf{a}'=\mathbf{a}-\mathbf{b},\quad \mathbf{b}'=\mathbf{a}+\mathbf{b},\quad \mathbf{c}'=\mathbf{c}$$
$$C_2 \text{ or } F_2\text{: (ii)}\quad \mathbf{a}'=\mathbf{a}+\mathbf{b},\quad \mathbf{b}'=-\mathbf{a}+\mathbf{b},\quad \mathbf{c}'=\mathbf{c}$$

(*cf.* Fig. 5.1.3.5). The secondary and tertiary symmetry directions are interchanged in the double cells. It is important to know how primary, secondary and tertiary symmetry elements change in the new cells $\mathbf{a}',\mathbf{b}',\mathbf{c}'$.

(i) *Primary symmetry elements*

In P groups, only two kinds of planes, m and n, occur perpendicular to the fourfold axis: a and b planes are forbidden. A plane m in the P cell corresponds to a plane in the C cell which has the character of both a mirror plane m and a glide plane n. This is due to the centring translation $\frac{1}{2},\frac{1}{2},0$ (*cf.* Chapter 4.1). Thus, the C-cell description shows† that $P4/m..$ (cell $\mathbf{a},\mathbf{b},\mathbf{c}$) has two maximal k subgroups of index [2], $P4/m..$ and $P4/n..$ (cells $\mathbf{a}',\mathbf{b}',\mathbf{c}'$), originating from the decentring of the C cell. The same reasoning is valid for $P4_2/m..$.

A glide plane n in the P cell is associated with glide planes a and b in the C cell. Since such planes do not exist in tetragonal P groups, the C cell cannot be decentred, *i.e.* $P4/n..$ and $P4_2/n..$ have no k subgroups of index [2] and cells $\mathbf{a}',\mathbf{b}',\mathbf{c}'$.

Glide planes a perpendicular to $\mathbf{c}$ only occur in $I4_1/a$ (88) and groups containing $I4_1/a$ [$I4_1/amd$ (141) and $I4_1/acd$ (142)]; they are associated with d planes in the F cell. These groups cannot be decentred, *i.e.* they have no P subgroups at all.

* For other g planes see (ii), *Secondary symmetry elements.*

† In this section, a dot stands for a symmetry element to be inserted in the corresponding position of the space-group symbol.

(ii) *Secondary symmetry elements*

In the tetragonal space-group symbols, one finds two kinds of secondary symmetry elements:

(1) 2, m, c without glide components in the ab plane occur in P and I groups. They transform to tertiary symmetry elements 2, m, c in the C or F cells, from which k subgroups can be obtained by decentring.

(2) $2_1, b, n$ with glide components $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $\frac{1}{2},\frac{1}{2},0$ in the ab plane occur only in P groups. In the C cell, they become tertiary symmetry elements with glide components $\frac{1}{4},-\frac{1}{4},0$; $\frac{1}{4},\frac{1}{4},0$; $\frac{1}{4},\frac{1}{4},\frac{1}{2}$. One has the following correspondence between P- and C-cell symbols:

$$P.2_1. = C..2_1$$
$$P.b. = C..g_1 \text{ with } g(\tfrac{1}{4},\tfrac{1}{4},0) \text{ in } \quad x,x-\tfrac{1}{4},z$$
$$P.n. = C..g_2 \text{ with } g(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{2}) \text{ in } \quad x,x-\tfrac{1}{4},z,$$

where $(g_1)^2$ and $(g_2)^2$ are the centring translations $\frac{1}{2},\frac{1}{2},0$ and $\frac{1}{2},\frac{1}{2},1$. Thus, the C cell cannot be decentred, *i.e.* tetragonal P groups having secondary symmetry elements 2_1, b or n cannot have *klassengleiche P* subgroups of index [2] and cells $\mathbf{a}',\mathbf{b}',\mathbf{c}'$.

(iii) *Tertiary symmetry elements*

Tertiary symmetry elements 2, m, c in P groups transform to secondary symmetry elements in the C cell, from which k subgroups can easily be deduced ($\rightarrow$):

$$\begin{array}{ccc} P..m = & C.m. \longrightarrow & P.m. \\ g & b & P.b. \\ P..c = & C.c. \longrightarrow & P.c. \\ n & n & P.n. \\ P..2 = & C.2. \longrightarrow & P.2. \\ 2_1 & 2_1 & P.2_1. \end{array}$$

Decentring leads in each case to two P subgroups (cell $\mathbf{a}',\mathbf{b}',\mathbf{c}'$), when allowed by (i) and (ii).

In I groups, 2, m and d occur as tertiary symmetry elements. They are transformed to secondary symmetry elements in the F cells. I groups with tertiary d glides cannot be decentred to P groups, whereas I groups with diagonal symmetry elements 2 and m have maximal P subgroups, due to decentring.

4.3.4.5. *Group–subgroup relations*

Examples are given for maximal k subgroups of P groups (i), of I groups (ii), and for maximal tetragonal, orthorhombic and monoclinic t subgroups.

4.3.4.5.1. *Maximal k subgroups*

(i) *Subgroups of P groups*

The discussion is limited to maximal P subgroups, obtained by decentring the larger C cell (*cf.* Section 4.3.4.4 *Multiple cells*).

Classes $\bar{4}$, 4 *and* 422

Examples

(1) Space groups $P\bar{4}$ (81) and $P4_p$ $(p = 0,1,2,3)$ (75–78) have isomorphic k subgroups of index [2], cell $\mathbf{a}',\mathbf{b}',\mathbf{c}'$.

(2) Space groups $P4_p22$ $(p = 0,1,2,3)$ (89, 91, 93, 95) have the extended C-cell symbol $\begin{matrix} C4_p2\ 2 \\ 2_1 \end{matrix}$, from which one deduces two k subgroups, $P4_p22$ (isomorphic, type **IIc**) and $P4_p2_12$ (non-isomorphic, type **IIb**), cell $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$.

(3) Space groups $P4_p2_12$ (90, 92, 94, 96) have no k subgroups of index [2], cell $\mathbf{a}',\mathbf{b}',\mathbf{c}'$.

Classes $\bar{4}m2$, $4mm$, $4/m$, *and* $4/mmm$

Examples

(1) $P\bar{4}c2$ (116) has the C-cell symbol $\begin{matrix} C\bar{4}2\ c \\ 2_1 \end{matrix}$, wherefrom one deduces two k subgroups, $P\bar{4}2c$ and $P\bar{4}2_1c$, cell $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$.

(2) $P4_2mc$ (105) has the C-cell symbol $\begin{matrix} C4_2cm \\ n \end{matrix}$, from which the k subgroups $P4_2cm$ (101) and $P4_2nm$ (102), cell $\mathbf{a}',\mathbf{b}',\mathbf{c}'$, are obtained.

(3) $P4_2/mcm$ (132) has the extended C symbol $\begin{matrix} C4_2/mmc \\ n\ b \end{matrix}$, wherefrom one reads the following k subgroups of index [2], cell $\mathbf{a}',\mathbf{b}',\mathbf{c}'$: $P4_2/mmc$, $P4_2/mbc$, $P4_2/nmc$, $P4_2/nbc$.

(4) $P4/nbm$ (125) has the extended C symbol $\begin{matrix} C4/amg_1 \\ bb \end{matrix}$ and has *no* k subgroups of index [2], as explained above in Section 4.3.4.4.

(ii) *Subgroups of I groups*

Note that I groups with a glides perpendicular to [001] or with diagonal d planes cannot be decentred (*cf.* above). The discussion is limited to P subgroups of index [2], obtained by decentring the I cell. These subgroups are easily read from the two-line symbols of the I groups in Table 4.3.2.1.

Examples

(1) $I4cm$ (108) has the extended symbol $\begin{matrix} I4\ ce \\ 4_2bm \end{matrix}$. The multiplication rules $4 \times b = m = 4_2 \times c$ give rise to the maximal k subgroups: $P4cc$, $P4_2bc$, $P4bm$, $P4_2cm$.

Similarly, $I4mm$ (107) has the P subgroups $P4mm$, $P4_2nm$, $P4nc$, $P4_2mc$, *i.e.* $I4mm$ and $I4cm$ have all P groups of class $4mm$ as maximal k subgroups.

(2) $I4/mcm$ (140) has the extended symbol $\begin{matrix} I4/m\ ce \\ 4_2/nbm \end{matrix}$. One obtains the subgroups of example (1) with an additional m or n plane perpendicular to $\mathbf{c}$.

As in example (1), $I4/mcm$ (140) and $I4/mmm$ (139) have all P groups of class $4/mmm$ as maximal k subgroups.

4.3.4.5.2. *Maximal t subgroups*

(i) *Tetragonal subgroups*

The class $4/mmm$ contains the classes $4/m, 422, 4mm$ and $\bar{4}2m$. Maximal t subgroups belonging to these classes are read directly from the standard full symbol.

Examples

(1) $P4_2/m\,bc$ (135) has the full symbol $P4_2/m\,2_1/b\,2/c$ and the tetragonal maximal t subgroups: $P4_2/m$, $P4_22_12$, $P4_2bc$, $P\bar{4}2_1c$, $P\bar{4}b2$.

(2) $I4/m\,cm$ (140) has the extended full symbol $\begin{matrix} I4/m\,2/c\ 2/e \\ 4_2/n\,2_1/b\,2_1/m \end{matrix}$ and the tetragonal maximal t subgroups $I4/m$, $I422$, $I4cm$, $I\bar{4}2m$, $I\bar{4}c2$. Note that the t subgroups of class $\bar{4}m2$ always exist in pairs.

(ii) *Orthorhombic subgroups*

In the orthorhombic subgroups, the symmetry elements belonging to directions [100] and [010] are the same, except that a glide plane b perpendicular to [100] is accompanied by a glide plane a perpendicular to [010].

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 $F\begin{matrix} b & a & n \\ c & c & m \\ m & m & n \end{matrix}$ ($Fmmm$), 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

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