(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 $\begin{array}{l} C4_p2\;2 \\ \quad\;\; 2_1 \end{array}$, 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 $\begin{array}{l} C\bar{4}2\;c \\ \quad\;\; 2_1 \end{array}$, 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 $\begin{array}{l} C4_2cm \\ \quad\;\; n \end{array}$, 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 $\begin{array}{l} C4_2/mmc \\ \qquad\;\; n\; b \end{array}$, 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 $\begin{array}{l} C4/amg_1 \\ \qquad bb \end{array}$ 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 $\begin{array}{l} I4\;\;ce \\ \;\;4_2bm \end{array}$. 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 $\begin{array}{l} I4/m\;ce \\ \;\;4_2/nbm \end{array}$. 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 $\begin{array}{l} I4/m\,2/c\;\;2/e \\ \;\;4_2/n\,2_1/b\,2_1/m \end{array}$ 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].

references