International Tables for Crystallography (2006). Vol. A, Section 4.3.3.2.2, p. 71.

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 $\begin{matrix} ccn \\ \text{class } mm2\text{: } Iba2;\ Ib2_1m\ (Ima2);\ I2_1am\ (Ima2). \end{matrix}$

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 $\begin{matrix} bna \\ \text{class } mm2\text{: } Cmc2_1;\ Cm2e\ (Aem2);\ C2ce\ (Aea2). \end{matrix}$

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.

references