*International Tables for Crystallography* (2006). Vol. A, Section 4.3.3.2, pp. 70–71.



the short Hermann–Mauguin symbols of *IT* (1935) for all space groups of class *mm*2, but was restored in *IT* (1952). In space groups of class 222, the last symmetry element cannot be omitted (see examples below).

For the new 'double' glide plane symbol '*e*', see the *Foreword to the Fourth Edition* (*IT* 1995) and Section 1.3.2, Note (x).

### 4.3.3.2. *Group–subgroup relations*

The present section emphasizes the use of the extended and full symbols for the derivation of maximal subgroups of types **I** and **IIa**; maximal orthorhombic subgroups of types **IIb** and **IIc** cannot be recognized by inspection of the synoptic Table 4.3.2.1.

#### 4.3.3.2.1. *Maximal non-isomorphic k subgroups of type* **IIa** *(decentred)*

(i) *Extended symbols of centred groups A, B, C, I*

By convention, the second line of the extended space-group symbol is the result of the multiplication of the first line by the centring translation (*cf.* Table 4.1.2.3). As a consequence, the product of any two terms in one line is equal to the product of the corresponding two terms in the other line.

(*a*) *Class* 222

The extended symbol of *I*222 (23) is $\begin{matrix} I2\ 2\ 2 \\ 2_12_12_1 \end{matrix}$; the twofold axes intersect and one obtains $2_x \times 2_y = 2_z = 2_{1x} \times 2_{1y}$.

Maximal *k* subgroups are *P*222 and $P2_12_12$ (plus permutations) but *not* $P2_12_12_1$.

The extended symbol of $I2_12_12_1$ (24) is $\begin{matrix} I2_12_12_1 \\ 2\ 2\ 2 \end{matrix}$, where one obtains $2_{1x} \times 2_{1y} = 2_{1z} = 2_x \times 2_y$; the twofold axes do *not* intersect. Thus, maximal non-isomorphic *k* subgroups are $P2_12_12_1$ and $P222_1$ (plus permutations), but *not* *P*222.

(*b*) *Class mm*2

The extended symbol of *Aea*2 (41) is $\begin{matrix} Aba2 \\ cn2_1 \end{matrix}$; the following relations hold: $b \times a = 2 = c \times n$ and $b \times n = 2_1 = c \times a$.

Maximal *k* subgroups are *Pba*2; *Pcn*2 (*Pnc*2); $Pbn2_1$ ($Pna2_1$); $Pca2_1$.

(*c*) *Class mmm*

By convention, the first line of the extended symbol contains those symmetry elements for which the coordinate triplets are explicitly printed under *Positions.* From the two-line symbols, as defined in the example below, one reads not only the eight maximal *k* subgroups *P* of class *mmm* but also the location of their centres of symmetry, by applying the following rules:

If in the symbol of the *P* subgroup the number of symmetry planes, chosen from the first line of the extended symbol, is odd (three or one), the symmetry centre is at 0, 0, 0; if it is even (two or zero), the symmetry centre is at $\frac{1}{4}, \frac{1}{4}, 0$ for the subgroups of *C* groups and at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ for the subgroups of *I* groups (Bertaut, 1976).

*Examples*

(1) According to these rules, the extended symbol of *Cmce* (64) is $\begin{matrix} Cmcb \\ bna \end{matrix}$ (see above). The four *k* subgroups with symmetry centres at 0, 0, 0 are *Pmcb* (*Pbam*); *Pmna*; *Pbca*; *Pbnb* (*Pccn*); those with symmetry centres at $\frac{1}{4}, \frac{1}{4}, 0$ are *Pbna* (*Pbcn*); *Pmca* (*Pbcm*); *Pmnb* (*Pnma*); *Pbcb* (*Pcca*). These rules can easily be transposed to other settings.

(2) The extended symbol of *Ibam* (72) is $\begin{matrix} Ibam \\ ccn \end{matrix}$. The four subgroups with symmetry centre at 0, 0, 0 are *Pbam*; *Pbcn*; *Pcan* (*Pbcn*); *Pccm*;
those with symmetry centre at $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ are *Pccn*; *Pcam* (*Pbcm*); *Pbcm*; *Pban.*

(ii) *Extended symbols of F-centred space groups*

Maximal *k* subgroups of the groups *F*222, *Fmm*2 and *Fmmm* are *C*, *A* and *B* groups. The corresponding centring translations are $w = t(\frac{1}{2}, \frac{1}{2}, 0), u = t(0, \frac{1}{2}, \frac{1}{2})$ and $v = w \times u = t(\frac{1}{2}, 0, \frac{1}{2})$.

The (four-line) extended symbols of these groups can be obtained from the following scheme:

| | *F*222 (22) | *Fmm*2 (42) | *Fmmm* (69) |
|---|---|---|---|
| 1 | 222 | *mm*2 | *mmm* |
| *w* | $2_12_12^w$ | $ba2^w$ | *ban* |
| *u* | $2^u2_12_1$ | $nc2_1$ | *ncb* |
| *v* | $2_1^u2^v2_1^w$ | $cn2_1^w$ | *cna* |

The second, third, and fourth lines are the result of the multiplication of the first line by the centring translations *w*, *u* and *v*, respectively.

The following abbreviations are used:

$$2_z^w = w \times 2_z; \quad 2_{1z}^w = w \times 2_{1z}; \; etc.$$

For the location of the symmetry elements in the above scheme, see Table 4.1.2.3. In Table 4.3.2.1, the centring translations and the superscripts *u*, *v*, *w* have been omitted. The first two lines of the scheme represent the extended symbols of *C*222, *Cmm*2 and *Cmmm.* An interchange of the symmetry elements in the first two lines does not change the group. To obtain further maximal *C* subgroups, one has to replace symmetry elements of the first line by corresponding elements of the third or fourth line. Note that the symbol '*e*' is not used in the four-line symbols for *Fmm*2 and *Fmmm* in order to keep the above scheme transparent.

*Examples*

(1) *F*222 (22). In the first line replace $2_x$ by $2_x^u$ (third line, same column) and keep $2_y$. Complete the first line by the product $2_x^u \times 2_y = 2_{1z}$ and obtain the maximal *C* subgroup $C2^u22_1$.

Similarly, in the first line keep $2_x$ and replace $2_y$ with $2_y^v$ (fourth line, same column). Complete the first line by the product $2_x \times 2_y^v = 2_{1z}$ and obtain the maximal *C* subgroup $C22^v2_1$.

Finally, replace $2_x$ and $2_y$ by $2_x^u$ and $2_y^v$ and form the product $2_x^u \times 2_y^v = 2_z^w$, to obtain the maximal *C* subgroup $C2^u2^v2^w$ (where $2^w$ can be replaced by 2). Note that *C*222 and $C2^u2^v2$ are two different subgroups, as are $C2^u22_1$ and $C22^v2_1$.

(2) *Fmm*2 (42). A similar procedure leads to the four maximal *k* subgroups *Cmm*2; $Cmc2_1$; $Ccm2_1^w$ ($Cmc2_1$); and *Ccc*2.

(3) *Fmmm* (69). One finds successively the eight maximal *k* subgroups *Cmmm*; *Cmma*; *Cmcm*; *Ccmm* (*Cmcm*); *Cmca*; *Ccma* (*Cmca*); *Cccm*; and *Ccca.*

Maximal *A*- and *B*-centred subgroups can be obtained from the *C* subgroups by simple symmetry arguments.

In space groups *Fdd*2 (43) and *Fddd* (70), the nature of the *d* planes is not altered by the translations of the *F* lattice; for this reason, a two-line symbol for *Fdd*2 and a one-line symbol for *Fddd* are sufficient. There exist no maximal non-isomorphic *k* subgroups for these two groups.



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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 class $mm2$: $Iba2$; $Ib2_1m$ ($Ima2$); $I2_1am$ ($Ima2$).
*ccn*

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 class $mm2$: $Cmc2_1$; $Cm2e$ ($Aem2$); $C2ce$ ($Aea2$).
*bna*

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 'l' 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 **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