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 $\begin{array}{c} I2\;2\;2 \\ 2_12_12_1 \end{array}$; 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 $\begin{array}{c} I2_12_12_1 \\ 2\;2\;2 \end{array}$, 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 $\begin{array}{c} Aba2 \\ cn2_1 \end{array}$; 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 $\begin{array}{c} Cmcb \\ bna \end{array}$ (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 $\begin{array}{c} Ibam \\ ccn \end{array}$. 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	$2^u2_1^v2_1$	$nc2_1$	*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.

references