International Tables for Crystallography (2006). Vol. A, Section 4.3.3, pp. 68–71.

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

TRIGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann-Mauguin symbols for standard cell *P* or *R*			Triple cell *H*
		Short	Full	Extended	
143	C_3^1	$P3$			$H3$
144	C_3^2	$P3_1$			$H3_1$
145	C_3^3	$P3_2$			$H3_2$
146	C_3^4	$R3$		$R3$ $3_{1,2}$	
147	C_{3i}^1	$P\bar{3}$			$H\bar{3}$
148	C_{3i}^2	$R\bar{3}$		$R\bar{3}$ $3_{1,2}$	
149	D_3^1	$P312$		$P312$ 2_1	$H321$
150	D_3^2	$P321$		$P321$ 2_1	$H312$
151	D_3^3	$P3_112$		$P3_112$ 2_1	$H3_121$
152	D_3^4	$P3_121$		$P3_121$ 2_1	$H3_112$
153	D_3^5	$P3_212$		$P3_212$ 2_1	$H3_221$
154	D_3^6	$P3_221$		$P3_221$ 2_1	$H3_212$
155	D_3^7	$R32$		$R3\ \ 2$ $3_{1,2}2_1$	
156	C_{3v}^1	$P3m1$		$P3m1$ b	$H31m$
157	C_{3v}^2	$P31m$		$P31m$ a	$H3m1$
158	C_{3v}^3	$P3c1$		$P3c1$ n	$H31c$
159	C_{3v}^4	$P31c$		$P31c$ n	$H3c1$
160	C_{3v}^5	$R3m$		$R3\ \ m$ $3_{1,2}b$	
161	C_{3v}^6	$R3c$		$R3\ \ c$ $3_{1,2}n$	
162	D_{3d}^1	$P\bar{3}1m$	$P\bar{3}12/m$	$P\bar{3}12/m$ $2_1/a$	$H\bar{3}m1$
163	D_{3d}^2	$P\bar{3}1c$	$P\bar{3}12/c$	$P\bar{3}12/c$ $2_1/n$	$H\bar{3}c1$
164	D_{3d}^3	$P\bar{3}m1$	$P\bar{3}2/m1$	$P\bar{3}2/m1$ $2_1/b$	$H\bar{3}1m$
165	D_{3d}^4	$P\bar{3}c1$	$P\bar{3}2/c1$	$P\bar{3}2/c1$ $2_1/n$	$H\bar{3}1c$
166	D_{3d}^5	$R\bar{3}m$	$R\bar{3}2/m$	$R\bar{3}\ \ 2/m$ $3_{1,2}2_1/b$	
167	D_{3d}^6	$R\bar{3}c$	$R\bar{3}2/c$	$R\bar{3}\ \ 2/c$ $3_{1,2}2_1/n$	

HEXAGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell *P*			Triple cell *H*
		Short	Full	Extended	
168	C_6^1	$P6$			$H6$
169	C_6^2	$P6_1$			$H6_1$
170	C_6^3	$P6_5$			$H6_5$
171	C_6^4	$P6_2$			$H6_2$
172	C_6^5	$P6_4$			$H6_4$
173	C_6^6	$P6_3$			$H6_3$
174	C_{3h}^1	$P\bar{6}$			$H\bar{6}$
175	C_{6h}^1	$P6/m$			$H6/m$
176	C_{6h}^2	$P6_3/m$			$H6_3/m$
177	D_6^1	$P622$		$P62\ 2$ 2_12_1	$H622$
178	D_6^2	$P6_122$		$P6_12\ 2$ 2_12_1	$H6_122$
179	D_6^3	$P6_522$		$P6_52\ 2$ 2_12_1	$H6_522$
180	D_6^4	$P6_222$		$P6_22\ 2$ 2_12_1	$H6_222$
181	D_6^5	$P6_422$		$P6_42\ 2$ 2_12_1	$H6_422$
182	D_6^6	$P6_322$		$P6_32\ 2$ 2_12_1	$H6_322$
183	C_{6v}^1	$P6mm$		$P6mm$ ba	$H6mm$
184	C_{6v}^2	$P6cc$		$P6cc$ nn	$H6cc$
185	C_{6v}^3	$P6_3cm$		$P6_3cm$ na	$H6_3mc$
186	C_{6v}^4	$P6_3mc$		$P6_3mc$ bn	$H6_3cm$
187	D_{3h}^1	$P\bar{6}m2$		$P\bar{6}m2$ $b2_1$	$H\bar{6}2m$
188	D_{3h}^2	$P\bar{6}c2$		$P\bar{6}c2$ $n2_1$	$H\bar{6}2c$
189	D_{3h}^3	$P\bar{6}2m$		$P\bar{6}2m$ 2_1a	$H\bar{6}m2$
190	D_{3h}^4	$P\bar{6}2c$		$P\bar{6}2\ \ c$ 2_1n	$H\bar{6}c2$
191	D_{6h}^1	$P6/mmm$	$P6/m2/m2/m$	$P6/m\,2/m\ 2/m$ $2_1/b\,2_1/a$	$H6/mmm$
192	D_{6h}^2	$P6/mcc$	$P6/m2/c2/c$	$P6/m\,2/c\ \ 2/c$ $2_1/n\,2_1/n$	$H6/mcc$
193	D_{6h}^3	$P6_3/mcm$	$P6_3/m2/c2/m$	$P6_3/m\,2/c\ \ 2/m$ $2_1/b\,2_1/a$	$H6_3/mmc$
194	D_{6h}^4	$P6_3/mmc$	$P6_3/m2/m2/c$	$P6_3/m\,2/m\ 2/c$ $2_1/b\,2_1/n$	$H6_3/mcm$

Example: $B\ 2/b\ 11$ (15, unique axis *a*)
$\quad 2_1/n$

The *t* subgroups of index [2] (type **I**) are $B211(C2)$; $Bb11(Cc)$; $B\bar{1}(P\bar{1})$.

The *k* subgroups of index [2] (type **IIa**) are $P2/b11(P2/c)$: $P2_1/b11(P2_1/c)$; $P2/n11(P2/c)$; $P2_1/n11(P2_1/c)$.

Some subgroups of index [4] (not maximal) are $P211(P2)$; $P2_111(P2_1)$; $Pb11(Pc)$; $Pn11(Pc)$; $P\bar{1}$; $B1(P1)$.

4.3.3. Orthorhombic system

4.3.3.1. *Historical note and arrangement of the tables*

The synoptic table of *IT* (1935) contained space-group symbols for the six orthorhombic 'settings', corresponding to the six permutations of the basis vectors **a**, **b**, **c**. In *IT* (1952), left-handed systems like $\bar{\mathbf{c}}\mathbf{ba}$ were changed to right-handed systems by reversing the orientation of the *c* axis, as in **cba**. Note that reversal

Table 4.3.2.1. *Index of symbols for space groups for various settings and cells* (*cont.*)

CUBIC SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols		
		Short	Full	Extended†
195	T^1	$P23$		
196	T^2	$F23$		$F23$ 2 2_1 2_1
197	T^3	$I23$		$I23$ 2_1
198	T^4	$P2_13$		
199	T^5	$I2_13$		$I2_13$ 2
200	T_h^1	$Pm\bar{3}$	$P2/m\bar{3}$	
201	T_h^2	$Pn\bar{3}$	$P2/n\bar{3}$	
202	T_h^3	$Fm\bar{3}$	$F/2m\bar{3}$	$F2/m\bar{3}$ $2/n$ $2_1/e$ $2_1/e$
203	T_h^4	$Fd\bar{3}$	$F2/d\bar{3}$	$F2/d\bar{3}$ $2/d$ $2_1/d$ $2_1/d$
204	T_h^5	$Im\bar{3}$	$I2/m\bar{3}$	$I2/m\bar{3}$ $2_1/n$
205	T_h^6	$Pa\bar{3}$	$P2_1/a\bar{3}$	
206	T_h^7	$Ia\bar{3}$	$I2_1/a\bar{3}$	$I2_1/a\bar{3}$ $2/b$
207	O^1	$P432$		$P4\ 32$ 2_1
208	O^2	$P4_232$		$P4_232$ 2_1
209	O^3	$F432$		$F4\ 32$ $4\ 2$ 4_22_1 4_22_1
210	O^4	$F4_132$		$F4_132$ $4_1\ 2$ $4_3\ 2_1$ $4_3\ 2_1$
211	O^5	$I432$		$I4\ 32$ $4_2\ 2_1$
212	O^6	$P4_332$		$P4_3\ 32$ 2_1
213	O^7	$P4_132$		$P4_132$ 2_1
214	O^8	$I4_132$		$I4_132$ $4_3\ 2_1$
215	T_d^1	$P\bar{4}3m$		$P\bar{4}3m$ g
216	T_d^2	$F\bar{4}3m$		$F\bar{4}3m$ g g_2 g_2
217	T_d^3	$I\bar{4}3m$		$I\bar{4}3m$ e
218	T_d^4	$P\bar{4}3n$		$P\bar{4}3n$ c
219	T_d^5	$F\bar{4}3c$		$F\bar{4}3n$ c g_1 g_1
220	T_d^6	$I\bar{4}3d$		$I\bar{4}3d$ d
221	O_h^1	$Pm\bar{3}m$	$P4/m\bar{3}2/m$	$P4/m\bar{3}2/m$ $2_1/g$
222	O_h^2	$Pn\bar{3}n$	$P4/n\bar{3}2/n$	$P4/n\bar{3}2/n$ $2_1/c$
223	O_h^3	$Pm\bar{3}n$	$P4_2/m\bar{3}2/n$	$P4_2/m\bar{3}2/n$ $2_1/c$
224	O_h^4	$Pn\bar{3}m$	$P4_2/n\bar{3}2/m$	$P4_2/n\bar{3}2/m$ $2_1/g$
225	O_h^5	$Fm\bar{3}m$	$F4/m\bar{3}2/m$	$F4/m\ \bar{3}2/m$ $4/n\ \ 2/g$ $4_2/e\ \ 2_1/g_2$ $4_2/e\ \ 2_1/g_2$
226	O_h^6	$Fm\bar{3}c$	$F4/m\bar{3}2/c$	$F4/m\bar{3}2/n$ $4/n\ 2/c$ $4_2/e\ 2_1/g_1$ $4_2/e\ 2_1/g_1$
227	O_h^7	$Fd\bar{3}m$	$F4_1/d\bar{3}2/m$	$F4_1/d\bar{3}2/m$ $4_1/d\ 2/g$ $4_3/d\ 2_1/g_2$ $4_3/d\ 2_1/g_2$
228	O_h^8	$Fd\bar{3}c$	$F4_1/d\bar{3}2/c$	$F4_1/d\bar{3}2/n$ $4_1/d\ 2/c$ $4_3/d\ 2_1/g_1$ $4_3/d\ 2_1/g_1$
229	O_h^9	$Im\bar{3}m$	$I4/m\bar{3}2/m$	$I4/m\bar{3}2/m$ $4_2/n\ 2_1/e$
230	O_h^{10}	$Ia\bar{3}d$	$I4_1/a\bar{3}2/d$	$I4_1/a\bar{3}2/d$ $4_3/b\ 2_1/d$

† Axes 3_1 and 3_2 parallel to axes 3 are not indicated in the extended symbols: *cf.* Chapter 4.1. For the glide-plane symbol '*e*', see the *Foreword to the Fourth Edition* (*IT* 1995) and Section 1.3.2, Note (x).

Note: The glide planes g, g_1 and g_2 have the glide components $g(\frac{1}{2}, \frac{1}{2}, 0)$, $g_1(\frac{1}{4}, \frac{1}{4}, 0)$ and $g_2(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$.

of two axes does not change the handedness of a coordinate system, so that the settings $\bar{\mathbf{c}}\mathbf{ba}$, $\mathbf{c}\bar{\mathbf{b}}\mathbf{a}$, $\mathbf{cb}\bar{\mathbf{a}}$ and $\bar{\mathbf{c}}\bar{\mathbf{b}}\bar{\mathbf{a}}$ are equivalent in this respect. The tabulation thus deals with the $6 \times 4 = 24$ possible right-handed settings. For further details see Section 2.2.6.4.

An important innovation of *IT* (1952) was the introduction of extended symbols for the centred groups *A*, *B*, *C*, *I*, *F*. These symbols are systematically developed in Table 4.3.2.1. Settings which permute the two axes **a** and **b** are listed side by side so that the two *C* settings appear together, followed by the two *A* and the two *B* settings.

In crystal classes *mm*2 and 222, the last symmetry element is the product of the first two and thus is not independent. It was omitted in 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	$2^u2_1^v2_1$	$nc2_1$	*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.

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.

references