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4.3. Symbols for space groups

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4.3.1. Triclinic system

There are only two triclinic space groups, $P1$ (1) and $P\bar{1}$ (2). $P1$ is quite outstanding because all its subgroups are also $P1$. They are listed in Table 13.2.2.1 for indices up to [7]. $P\bar{1}$ has subgroups $P\bar{1}$, isomorphic, and $P1$, non-isomorphic.

In the triclinic system, a primitive unit cell can always be selected. In some cases, however, it may be advantageous to select a larger cell, with A, B, C, I or F centring.

The two types of reduced bases (reduced cells) are discussed in Section 9.2.2.

4.3.2. Monoclinic system

4.3.2.1. *Historical note and arrangement of the tables*

In *IT* (1935) only the b axis was considered as the unique axis. In *IT* (1952) two choices were given: the c-axis setting was called the 'first setting' and the b-axis setting was designated the 'second setting'.

To avoid the presence of two standard space-group symbols side by side, in the present tables only *one standard short symbol* has been chosen, that conforming to the long-lasting tradition of the b-axis unique (*cf.* Sections 2.2.4 and 2.2.16). However, for reasons of rigour and completeness, in Table 4.3.2.1 the *full* symbols are given not only for the c-axis and the b-axis settings but also for the a-axis setting. Thus, Table 4.3.2.1 has six columns which in pairs refer to these three settings. In the headline, the unique axis of each setting is underlined.

Additional complications arise from the presence of fractional translations due to glide planes in the primitive cell [groups Pc (7), $P2/c$ (13), $P2_1/c$ (14)], due to centred cells [$C2$ (5), Cm (8), $C2/m$ (12)], or due to both [Cc (9), $C2/c$ (15)]. For these groups, three different choices of the two oblique axes are possible which are called 'cell choices' 1, 2 and 3 (see Section 2.2.16). If this is combined with the three choices of the unique axis, $3 \times 3 = 9$ symbols result. If we add the effect of the permutation of the two oblique axes (and simultaneously reversing the sense of the unique axis to keep the system right-handed, as in **abc** and $\mathbf{c\bar{b}a}$), we arrive at the $9 \times 2 = 18$ symbols listed in Table 4.3.2.1 for each of the eight space groups mentioned above.

The space-group symbols $P2$ (3), $P2_1$ (4), Pm (6), $P2/m$ (10) and $P2_1/m$ (11) do not depend on the cell choice: in these cases, one line of six space-group symbols is sufficient.

For space groups with centred lattices (A, B, C, I), extended symbols are given; the 'additional symmetry elements' (due to the centring) are printed in the half line below the space-group symbol.

The use of the present tabulation is illustrated by two examples, Pm, which does not depend on the cell choice, and $C2/c$, which does.

Examples

(1) Pm (6)

(i) *Unique axis b*

In the first column, headed by $\mathbf{a\underline{b}c}$, one finds the full symbol $P1m1$. Interchanging the labels of the oblique axes a and c does not change this symbol, which is found again in the second column headed by $\mathbf{c\underline{\bar{b}}a}$.

(ii) *Unique axis c*

In the third column, headed by $\mathbf{ab\underline{c}}$, one finds the symbol $P11m$. Again, this symbol is conserved in the interchange of the oblique axes a and b, as seen in the fourth column headed by $\mathbf{ba\underline{\bar{c}}}$.

The same applies to the setting with unique axis a, columns five and six.

(2) $C2/c$ (15)

The short symbol $C2/c$ is followed by three lines, corresponding to the cell choices 1, 2, 3. Each line contains six full space-group symbols.

(i) *Unique axis b*

The column headed by $\mathbf{a\underline{b}c}$ contains the three symbols $C\,1\,2/c\,1$, $A1\,2/n\,1$ and $I1\,2/a\,1$, equivalent to the short symbol $C2/c$ and corresponding to the cell choices 1, 2, 3. In the half line below each symbol, the additional symmetry elements are indicated (extended symbol). If the oblique axes a and c are interchanged, the column under $\mathbf{c\underline{b}a}$ lists the symbols $A1\,2/a\,1$, $C1\,2/n\,1$ and $I1\,2/c\,1$ for the three cell choices.

(ii) *Unique axis c*

The column under $\mathbf{ab\underline{c}}$ contains the symbols $A112/a$, $B112/n$ and $I112/b$, corresponding to the cell choices 1, 2 and 3. If the oblique axes a and b are interchanged, the column under $\mathbf{ba\underline{\bar{c}}}$ applies.

Similar considerations apply to the a-axis setting.

4.3.2.2. *Transformation of space-group symbols*

How does a monoclinic space-group symbol transform for the various settings of the same unit cell? This can be easily recognized with the help of the headline of Table 4.3.2.1, completed to the following scheme:

$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	**cab**	$\mathbf{ac\bar{b}}$	**bca**	$\mathbf{\bar{b}ac}$	Unique axis b
bca	$\mathbf{a\bar{c}b}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	**cab**	$\mathbf{\bar{c}ba}$	Unique axis c
cab	$\mathbf{b\bar{a}c}$	**bca**	$\mathbf{cb\bar{a}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	Unique axis a.

The use of this three-line scheme is illustrated by the following examples.

Examples

(1) $C2/c$ (15, unique axis b, cell choice 1)

Extended symbol: $C1\,2/c\,1$.
$2_1/n$

Consider the setting **cab**, first line, third column. Compared to the initial setting $\mathbf{a\underline{b}c}$, it contains the 'unique axis b' in the third place and, consequently, must be identified with the setting $\mathbf{ab\underline{c}}$, unique axis c, in the third column, for which in Table 4.3.2.1 the new symbol for cell choice 1 is listed as $A11\,2/a$
$2_1/n$.

(2) $C2/c$ (15, unique axis b, cell choice 3)

Extended symbol: $I1\,2/a\;\,1$.
$2_1/c$

Consider the setting $\mathbf{\bar{b}ac}$ in the first line, sixth column. It contains the 'unique axis b' in the first place and thus must be identified with the setting $\mathbf{\underline{\bar{a}}cb}$, unique axis a, in the sixth column. From Table 4.3.2.1, the appropriate space-group symbol for cell choice 3 is found as $I\;2/b\;11$.
$2_1/c$

4.3.2.3. *Group–subgroup relations*

It is easy to read all monoclinic maximal t and k subgroups of types **I** and **IIa** directly from the extended full symbols of a space group. Maximal subgroups of types **IIb** and **IIc** cannot be recognized by simple inspection of the synoptic Table 4.3.2.1

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

TRICLINIC SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbol for all settings of the same unit cell
1	C_1^1	$P1$
2	C_i^1	$P\bar{1}$

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						
			$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	Unique axis b Unique axis c Unique axis a
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121$ 2_1	$A121$ 2_1	$A112$ 2_1	$B112$ 2_1	$B211$ 2_1	$C211$ 2_1	Cell choice 1
			$A121$ 2_1	$C121$ 2_1	$B112$ 2_1	$A112$ 2_1	$C211$ 2_1	$B211$ 2_1	Cell choice 2
			$I121$ 2_1	$I121$ 2_1	$I112$ 2_1	$I112$ 2_1	$I211$ 2_1	$I211$ 2_1	Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$	$P1a1$	$P11a$	$P11b$	$Pb11$	$Pc11$	Cell choice 1
			$P1n1$	$P1n1$	$P11n$	$P11n$	$Pn11$	$Pn11$	Cell choice 2
			$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3
8	C_s^3	Cm	$C1m1$ a	$A1m1$ c	$A11m$ b	$B11m$ a	$Bm11$ c	$Cm11$ b	Cell choice 1
			$A1m1$ c	$C1m1$ a	$B11m$ a	$A11m$ b	$Cm11$ b	$Bm11$ c	Cell choice 2
			$I1m1$ n	$I1m1$ n	$I11m$ n	$I11m$ n	$Im11$ n	$Im11$ n	Cell choice 3
9	C_s^4	Cc	$C1c1$ n	$A1a1$ n	$A11a$ n	$B11b$ n	$Bb11$ n	$Cc11$ n	Cell choice 1
			$A1n1$ a	$C1n1$ c	$B11n$ b	$A11n$ a	$Cn11$ c	$Bn11$ b	Cell choice 2
			$I1a1$ c	$I1c1$ a	$I11b$ a	$I11a$ b	$Ic11$ b	$Ib11$ c	Cell choice 3
10	C_{2h}^1	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	C_{2h}^2	$P2_1/m$	$P1\frac{2_1}{m}1$	$P1\frac{2_1}{m}1$	$P11\frac{2_1}{m}$	$P11\frac{2_1}{m}$	$P\frac{2_1}{m}11$	$P\frac{2_1}{m}11$	
12	C_{2h}^3	$C2/m$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$	$A1\frac{2}{m}1$ $\frac{2_1}{c}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$	$B11\frac{2}{m}$ $\frac{2_1}{a}$	$B\frac{2}{m}11$ $\frac{2_1}{c}$	$C\frac{2}{m}11$ $\frac{2_1}{b}$	Cell choice 1
			$A1\frac{2}{m}1$ $\frac{2_1}{c}$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$	$B11\frac{2}{m}$ $\frac{2_1}{a}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$	$C\frac{2}{m}11$ $\frac{2_1}{b}$	$B\frac{2}{m}11$ $\frac{2_1}{c}$	Cell choice 2
			$I1\frac{2}{m}1$ $\frac{2_1}{n}$	$I1\frac{2}{m}1$ $\frac{2_1}{n}$	$I11\frac{2}{m}$ $\frac{2_1}{n}$	$I11\frac{2}{m}$ $\frac{2_1}{n}$	$I\frac{2}{m}11$ $\frac{2_1}{n}$	$I\frac{2}{m}11$ $\frac{2_1}{n}$	Cell choice 3
13	C_{2h}^4	$P2/c$	$P1\frac{2}{c}1$	$P1\frac{2}{a}1$	$P11\frac{2}{a}$	$P11\frac{2}{b}$	$P\frac{2}{b}11$	$P\frac{2}{c}11$	Cell choice 1
			$P1\frac{2}{n}1$	$P1\frac{2}{n}1$	$P11\frac{2}{n}$	$P11\frac{2}{n}$	$P\frac{2}{n}11$	$P\frac{2}{n}11$	Cell choice 2
			$P1\frac{2}{a}1$	$P1\frac{2}{c}1$	$P11\frac{2}{b}$	$P11\frac{2}{a}$	$P\frac{2}{c}11$	$P\frac{2}{b}11$	Cell choice 3

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

MONOCLINIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						
			$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	Unique axis *b* Unique axis *c* Unique axis *a*
14	C_{2h}^5	$P2_1/c$	$P1\frac{2_1}{c}1$	$P1\frac{2_1}{a}1$	$P11\frac{2_1}{a}$	$P11\frac{2_1}{b}$	$P\frac{2_1}{b}11$	$P\frac{2_1}{c}11$	Cell choice 1
			$P1\frac{2_1}{n}1$	$P1\frac{2_1}{n}1$	$P11\frac{2_1}{n}$	$P11\frac{2_1}{n}$	$P\frac{2_1}{n}11$	$P\frac{2_1}{n}11$	Cell choice 2
			$P1\frac{2_1}{a}1$	$P1\frac{2_1}{c}1$	$P11\frac{2_1}{b}$	$P11\frac{2_1}{a}$	$P\frac{2_1}{c}11$	$P\frac{2_1}{b}11$	Cell choice 3
15	C_{2h}^6	$C2/c$	$C1\frac{2}{c}1$ $\frac{2_1}{n}$	$A1\frac{2}{a}1$ $\frac{2_1}{n}$	$A11\frac{2}{a}$ $\frac{2_1}{n}$	$B11\frac{2}{b}$ $\frac{2_1}{n}$	$B\frac{2}{b}11$ $\frac{2_1}{n}$	$C\frac{2}{c}11$ $\frac{2_1}{n}$	Cell choice 1
			$A1\frac{2}{n}1$ $\frac{2_1}{a}$	$C1\frac{2}{n}1$ $\frac{2_1}{c}$	$B11\frac{2}{n}$ $\frac{2_1}{b}$	$A11\frac{2}{n}$ $\frac{2_1}{a}$	$C\frac{2}{n}11$ $\frac{2_1}{c}$	$B\frac{2}{n}11$ $\frac{2_1}{b}$	Cell choice 2
			$I1\frac{2}{a}1$ $\frac{2_1}{c}$	$I1\frac{2}{c}1$ $\frac{2_1}{a}$	$I11\frac{2}{b}$ $\frac{2_1}{a}$	$I11\frac{2}{a}$ $\frac{2_1}{b}$	$I\frac{2}{c}11$ $\frac{2_1}{b}$	$I\frac{2}{b}11$ $\frac{2_1}{c}$	Cell choice 3

ORTHORHOMBIC SYSTEM

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
		abc	**abc** (standard)	$\mathbf{ba\bar{c}}$	**cab**	$\mathbf{\bar{c}ba}$	**bca**	$\mathbf{a\bar{c}b}$
16	D_2^1	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$
17	D_2^2	$P222_1$	$P222_1$	$P222_1$	$P2_122$	$P2_122$	$P22_12$	$P22_12$
18	D_2^3	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P22_12_1$	$P22_12_1$	$P2_122_1$	$P2_122_1$
19	D_2^4	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
20	D_2^5	$C222_1$	$C222_1$ $2_12_12_1$	$C222_1$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$B22_12$ $2_12_12_1$	$B22_12$ $2_12_12_1$
21	D_2^6	$C222$	$C222$ 2_12_12	$C222$ 2_12_12	$A222$ 22_12_1	$A222$ 22_12_1	$B222$ 2_122_1	$B222$ 2_122_1
22	D_2^7	$F222$	$F222$ 2_12_12 22_12_1 2_122_1	$F222$ 2_12_12 2_122_1 22_12_1	$F222$ 22_12_1 2_122_1 2_12_12	$F222$ 22_12_1 2_12_12 2_122_1	$F222$ 2_122_1 2_12_12 22_12_1	$F222$ 2_122_1 22_12_1 2_12_12
23	D_2^8	$I222$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$
24	D_2^9	$I2_12_12_1$	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222
25	C_{2v}^1	$Pmm2$	$Pmm2$	$Pmm2$	$P2mm$	$P2mm$	$Pm2m$	$Pm2m$
26	C_{2v}^2	$Pmc2_1$	$Pmc2_1$	$Pcm2_1$	$P2_1ma$	$P2_1am$	$Pb2_1m$	$Pm2_1b$
27	C_{2v}^3	$Pcc2$	$Pcc2$	$Pcc2$	$P2aa$	$P2aa$	$Pb2b$	$Pb2b$
28	C_{2v}^4	$Pma2$	$Pma2$	$Pbm2$	$P2mb$	$P2cm$	$Pc2m$	$Pm2a$
29	C_{2v}^5	$Pca2_1$	$Pca2_1$	$Pbc2_1$	$P2_1ab$	$P2_1ca$	$Pc2_1b$	$Pb2_1a$
30	C_{2v}^6	$Pnc2$	$Pnc2$	$Pcn2$	$P2na$	$P2an$	$Pb2n$	$Pn2b$
31	C_{2v}^7	$Pmn2_1$	$Pmn2_1$	$Pnm2_1$	$P2_1mn$	$P2_1nm$	$Pn2_1m$	$Pm2_1n$
32	C_{2v}^8	$Pba2$	$Pba2$	$Pba2$	$P2cb$	$P2cb$	$Pc2a$	$Pc2a$
33	C_{2v}^9	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$
34	C_{2v}^{10}	$Pnn2$	$Pnn2$	$Pnn2$	$P2nn$	$P2nn$	$Pn2n$	$Pn2n$

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

ORTHORHOMBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	$\mathbf{ba\bar{c}}$	**cab**	$\mathbf{\bar{c}ba}$	**bca**	$\mathbf{a\bar{c}b}$
35	C_{2v}^{11}	*Cmm*2	*Cmm*2 *ba*2	*Cmm*2 *ba*2	*A*2*mm* 2*cb*	*A*2*mm* 2*cb*	*Bm*2*m* *c*2*a*	*Bm*2*m* *c*2*a*
36	C_{2v}^{12}	$Cmc2_1$	$Cmc2_1$ $bn2_1$	$Ccm2_1$ $na2_1$	$A2_1ma$ 2_1cn	$A2_1am$ 2_1nb	$Bb2_1m$ $n2_1a$	$Bm2_1b$ $c2_1n$
37	C_{2v}^{13}	*Ccc*2	*Ccc*2 *nn*2	*Ccc*2 *nn*2	*A*2*aa* 2*nn*	*A*2*aa* 2*nn*	*Bb*2*b* *n*2*n*	*Bb*2*b* *n*2*n*
38	C_{2v}^{14}	*Amm*2	*Amm*2 $nc2_1$	*Bmm*2 $cn2_1$	*B*2*mm* 2_1na	*C*2*mm* 2_1an	*Cm*2*m* $b2_1n$	*Am*2*m* $n2_1b$
39*	C_{2v}^{15}	*Aem*2	*Aem*2 $ec2_1$	*Bme*2 $ce2_1$	*B*2*em* 2_1ea	*C*2*me* 2_1ae	*Cm*2*e* $b2_1e$	*Ae*2*m* $e2_1b$
40	C_{2v}^{16}	*Ama*2	*Ama*2 $nn2_1$	*Bbm*2 $nn2_1$	*B*2*mb* 2_1nn	*C*2*cm* 2_1nn	*Cc*2*m* $n2_1n$	*Am*2*a* $n2_1n$
41*	C_{2v}^{17}	*Aea*2	*Aea*2 $en2_1$	*Bbe*2 $ne2_1$	*B*2*eb* 2_1en	*C*2*ce* 2_1ne	*Cc*2*e* $n2_1e$	*Ae*2*a* $e2_1n$
42	C_{2v}^{18}	*Fmm*2	*Fmm*2 *ba*2 $nc2_1$ $cn2_1$	*Fmm*2 *ba*2 $cn2_1$ $nc2_1$	*F*2*mm* 2*cb* 2_1na 2_1an	*F*2*mm* 2*cb* 2_1an 2_1na	*Fm*2*m* *c*2*a* $b2_1n$ $n2_1b$	*Fm*2*m* *c*2*a* $n2_1b$ $b2_1n$
43	C_{2v}^{19}	*Fdd*2	*Fdd*2 $dd2_1$	*Fdd*2 $dd2_1$	*F*2*dd* 2_1dd	*F*2*dd* 2_1dd	*Fd*2*d* $d2_1d$	*Fd*2*d* $d2_1d$
44	C_{2v}^{20}	*Imm*2	*Imm*2 $nn2_1$	*Imm*2 $nn2_1$	*I*2*mm* 2_1nn	*I*2*mm* 2_1nn	*Im*2*m* $n2_1n$	*Im*2*m* $n2_1n$
45	C_{2v}^{21}	*Iba*2	*Iba*2 $cc2_1$	*Iba*2 $cc2_1$	*I*2*cb* 2_1aa	*I*2*cb* 2_1aa	*Ic*2*a* $b2_1b$	*Ic*2*a* $b2_1b$
46	C_{2v}^{22}	*Ima*2	*Ima*2 $nc2_1$	*Ibm*2 $cn2_1$	*I*2*mb* 2_1na	*I*2*cm* 2_1an	*Ic*2*m* $b2_1n$	*Im*2*a* $n2_1b$
47	D_{2h}^{1}	$P\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*
48	D_{2h}^{2}	$P\frac{2}{n}\frac{2}{n}\frac{2}{n}$	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*
49	D_{2h}^{3}	$P\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Pccm*	*Pccm*	*Pmaa*	*Pmaa*	*Pbmb*	*Pbmb*
50	D_{2h}^{4}	$P\frac{2}{b}\frac{2}{a}\frac{2}{n}$	*Pban*	*Pban*	*Pncb*	*Pncb*	*Pcna*	*Pcna*
51	D_{2h}^{5}	$P\frac{2_1}{m}\frac{2}{m}\frac{2}{a}$	*Pmma*	*Pmmb*	*Pbmm*	*Pcmm*	*Pmcm*	*Pmam*
52	D_{2h}^{6}	$P\frac{2}{n}\frac{2_1}{n}\frac{2}{a}$	*Pnna*	*Pnnb*	*Pbnn*	*Pcnn*	*Pncn*	*Pnan*
53	D_{2h}^{7}	$P\frac{2}{m}\frac{2}{n}\frac{2_1}{a}$	*Pmna*	*Pnmb*	*Pbmn*	*Pcnm*	*Pncm*	*Pman*
54	D_{2h}^{8}	$P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$	*Pcca*	*Pccb*	*Pbaa*	*Pcaa*	*Pbcb*	*Pbab*
55	D_{2h}^{9}	$P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$	*Pbam*	*Pbam*	*Pmcb*	*Pmcb*	*Pcma*	*Pcma*
56	D_{2h}^{10}	$P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$	*Pccn*	*Pccn*	*Pnaa*	*Pnaa*	*Pbnb*	*Pbnb*
57	D_{2h}^{11}	$P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}$	*Pbcm*	*Pcam*	*Pmca*	*Pmab*	*Pbma*	*Pcmb*
58	D_{2h}^{12}	$P\frac{2_1}{n}\frac{2_1}{n}\frac{2}{m}$	*Pnnm*	*Pnnm*	*Pmnn*	*Pmnn*	*Pnmn*	*Pnmn*
59	D_{2h}^{13}	$P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}$	*Pmmn*	*Pmmn*	*Pnmm*	*Pnmm*	*Pmnm*	*Pmnm*
60	D_{2h}^{14}	$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$	*Pbcn*	*Pcan*	*Pnca*	*Pnab*	*Pbna*	*Pcnb*
61	D_{2h}^{15}	$P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*Pbca*	*Pcab*	*Pbca*	*Pcab*	*Pbca*	*Pcab*

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

ORTHORHOMBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**ba$\bar{\mathbf{c}}$**	**cab**	**$\bar{\mathbf{c}}$ba**	**bca**	**a$\bar{\mathbf{c}}$b**
62	D_{2h}^{16}	$P\,\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	*Pnma*	*Pmnb*	*Pbnm*	*Pcmn*	*Pmcn*	*Pnam*
63	D_{2h}^{17}	$C\,\frac{2}{m}\frac{2}{c}\frac{2_1}{m}$	*Cmcm* *bnn*	*Ccmm* *nan*	*Amma* *ncn*	*Amam* *nnb*	*Bbmm* *nna*	*Bmmb* *cnn*
64*†	D_{2h}^{18}	$C\,\frac{2}{m}\frac{2}{c}\frac{2_1}{e}$	*Cmce* *bne*	*Ccme* *nae*	*Aema* *ecn*	*Aeam* *enb*	*Bbem* *nea*	*Bmeb* *cen*
65	D_{2h}^{19}	$C\,\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Cmmm* *ban*	*Cmmm* *ban*	*Ammm* *ncb*	*Ammm* *ncb*	*Bmmm* *cna*	*Bmmm* *cna*
66	D_{2h}^{20}	$C\,\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Cccm* *nnn*	*Cccm* *nnn*	*Amaa* *nnn*	*Amaa* *nnn*	*Bbmb* *nnn*	*Bbmb* *nnn*
67*†	D_{2h}^{21}	$C\,\frac{2}{m}\frac{2}{m}\frac{2}{e}$	*Cmme* *bae*	*Cmme* *bae*	*Aemm* *ecb*	*Aemm* *ecb*	*Bmem* *cea*	*Bmem* *cea*
68*	D_{2h}^{22}	$C\,\frac{2}{c}\frac{2}{c}\frac{2}{e}$	*Ccce* *nne*	*Ccce* *nne*	*Aeaa* *enn*	*Aeaa* *enn*	*Bbeb* *nen*	*Bbeb* *nen*
69	D_{2h}^{23}	$F\,\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Fmmm* *ban* *ncb* *cna*	*Fmmm* *ban* *cna* *ncb*	*Fmmm* *ncb* *cna* *ban*	*Fmmm* *ncb* *ban* *cna*	*Fmmm* *cna* *ban* *ncb*	*Fmmm* *cna* *ncb* *ban*
70	D_{2h}^{24}	$F\,\frac{2}{d}\frac{2}{d}\frac{2}{d}$	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*
71	D_{2h}^{25}	$I\,\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*
72	D_{2h}^{26}	$I\,\frac{2}{b}\frac{2}{a}\frac{2}{m}$	*I bam* *ccn*	*I bam* *ccn*	*I mcb* *naa*	*I mcb* *naa*	*I cma* *bnb*	*I cma* *bnb*
73	D_{2h}^{27}	$I\,\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*
74†	D_{2h}^{28}	$I\,\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}$	*I mma* *nnb*	*I mmb* *nna*	*I bmm* *cnn*	*I cmm* *bnn*	*I mcm* *nan*	*I mam* *ncn*

* For the five space groups *Aem*2 (39), *Aea*2 (41), *Cmce* (64), *Cmme* (67) and *Ccce* (68), the 'new' space-group symbols, containing the symbol '*e*' for the 'double' glide plane, are given for all settings. These symbols were first introduced in the Fourth Edition of this volume (*IT* 1995); *cf. Foreword to the Fourth Edition.* For further explanations, see Section 1.3.2, Note (x) and the space-group diagrams.

† For space groups *Cmca* (64), *Cmma* (67) and *Imma* (74), the first lines of the extended symbols, as tabulated here, correspond with the symbols for the six settings in the diagrams of these space groups (Part 7). An alternative formulation which corresponds with the coordinate triplets is given in Section 4.3.3.

TETRAGONAL SYSTEM

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell *P* or *I*		Multiple cell *C* or *F*	
		Short	Extended	Short	Extended
75	C_4^1	$P4$		$C4$	
76	C_4^2	$P4_1$		$C4_1$	
77	C_4^3	$P4_2$		$C4_2$	
78	C_4^4	$P4_3$		$C4_3$	
79	C_4^5	$I\,4$	$I4$ 4_2	$F4$	$F4$ 4_2
80	C_4^6	$I\,4_1$	$I4_1$ 4_3	$F4_1$	$F4_1$ 4_3
81	S_4^1	$P\bar{4}$		$C\bar{4}$	
82	S_4^2	$I\bar{4}$		$F\bar{4}$	

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell *P* or *I*		Multiple cell *C* or *F*	
		Short	Extended	Short	Extended
83	C_{4h}^1	$P4/m$		$C4/m$	$C4_2/m$ n
84	C_{4h}^2	$P4_2/m$		$C4_2/m$	$C4_2/m$ n
85	C_{4h}^3	$P4/n$		$C4/a$	$C4/a$ b
86	C_{4h}^4	$P4_2/n$		$C4_2/a$	$C4_2/a$ b
87	C_{4h}^5	$I\,4/m$	$I4/m$ $4_2/n$	$F4/m$	$F4/m$ $4_2/a$
88	C_{4h}^6	$I\,4_1/a$	$I4_1/a$ $4_3/b$	$F4_1/d$	$F4_1/d$ $4_3/d$

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

TETRAGONAL SYSTEM (*cont.*)

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell *P* or *I*		Multiple cell *C* or *F*	
		Short	Extended	Short	Extended
89	D_4^1	$P422$	$P422$ 2_1	$C422$	$C422$ 2_1
90	D_4^2	$P42_12$	$P42_12$ 2_1	$C422_1$	$C422_1$ 2_1
91	D_4^3	$P4_122$	$P4_122$ 2_1	$C4_122$	$C4_122$ 2_1
92	D_4^4	$P4_12_12$	$P4_12_12$ 2_1	$C4_122_1$	$C4_122_1$ 2_1
93	D_4^5	$P4_222$	$P4_222$ 2_1	$C4_222$	$C4_222$ 2_1
94	D_4^6	$P4_22_12$	$P4_22_12$ 2_1	$C4_222_1$	$C4_222_1$ 2_1
95	D_4^7	$P4_322$	$P4_322$ 2_1	$C4_322$	$C4_322$ 2_1
96	D_4^8	$P4_32_12$	$P4_32_12$ 2_1	$C4_322_1$	$C4_322_1$ 2_1
97	D_4^9	$I422$	$I422$ $4_22_12_1$	$F422$	$F422$ $4_22_12_1$
98	D_4^{10}	$I4_122$	$I4_122$ $4_32_12_1$	$F4_122$	$F4_122$ $4_32_12_1$
99	C_{4v}^1	$P4mm$	$P4mm$ g	$C4mm$	$C4mm$ b
100	C_{4v}^2	$P4bm$	$P4bm$ g	$C4mg_1$	$C4mg_1$ b
101	C_{4v}^3	$P4_2cm$	$P4_2cm$ g	$C4_2mc$	$C4_2mc$ b
102	C_{4v}^4	$P4_2nm$	$P4_2nm$ g	$C4_2mg_2$	$C4_2mg_2$ b
103	C_{4v}^5	$P4cc$	$P4cc$ n	$C4cc$	$C4cc$ n
104	C_{4v}^6	$P4nc$	$P4nc$ n	$C4cg_2$	$C4cg_2$ n
105	C_{4v}^7	$P4_2mc$	$P4_2mc$ n	$C4_2cm$	$C4_2cm$ n
106	C_{4v}^8	$P4_2bc$	$P4_2bc$ n	$C4_2cg_1$	$C4_2cg_1$ n
107	C_{4v}^9	$I4mm$	$I4mm$ 4_2ne	$F4mm$	$F4mm$ 4_2eg_2
108	C_{4v}^{10}	$I4cm$	$I4ce$ 4_2bm	$F4mc$	$F4ec$ 4_2mg_1
109	C_{4v}^{11}	$I4_1md$	$I4_1md$ 4_1nd	$F4_1dm$	$F4_1dm$ 4_3dg_2
110	C_{4v}^{12}	$I4_1cd$	$I4_1cd$ 4_3bd	$F4_1dc$	$F4_1dc$ 4_3dg_1
111	D_{2d}^1	$P\bar{4}2m$	$P\bar{4}2m$ g	$C\bar{4}m2$	$C\bar{4}m2$ b
112	D_{2d}^2	$P\bar{4}2c$	$P\bar{4}2c$ n	$C\bar{4}c2$	$C\bar{4}c2$ n
113	D_{2d}^3	$P\bar{4}2_1m$	$P\bar{4}2_1m$ g	$C\bar{4}m2_1$	$C\bar{4}m2_1$ b
114	D_{2d}^4	$P\bar{4}2_1c$	$P\bar{4}2_1c$ n	$C\bar{4}c2_1$	$C\bar{4}c2_1$ n
115	D_{2d}^5	$P\bar{4}m2$	$P\bar{4}m2$ 2_1	$C\bar{4}2m$	$C\bar{4}2m$ 2_1
116	D_{2d}^6	$P\bar{4}c2$	$P\bar{4}c2$ 2_1	$C\bar{4}2c$	$C\bar{4}2c$ 2_1
117	D_{2d}^7	$P\bar{4}b2$	$P\bar{4}b2$ 2_1	$C\bar{4}2g_1$	$C\bar{4}2g_1$ 2_1
118	D_{2d}^8	$P\bar{4}n2$	$P\bar{4}n2$ 2_1	$C\bar{4}2g_2$	$C\bar{4}2g_2$ 2_1

TETRAGONAL SYSTEM (*cont.*)

No. of space group	Schoen-flies symbol	Hermann–Mauguin symbols for standard cell *P* or *I*		Multiple cell *C* or *F*	
		Short	Extended	Short	Extended
119	D_{2d}^9	$I\bar{4}m2$	$I\bar{4}m2$ $n2_1$	$F\bar{4}2m$	$F\bar{4}2m$ 2_1g_2
120	D_{2d}^{10}	$I\bar{4}c2$	$I\bar{4}c2$ $b2_1$	$F\bar{4}2c$	$F\bar{4}2c$ 2_1n
121	D_{2d}^{11}	$I\bar{4}2m$	$I\bar{4}2m$ 2_1e	$F\bar{4}m2$	$F\bar{4}m2$ $e2_1$
122	D_{2d}^{12}	$I\bar{4}2d$	$I\bar{4}2d$ 2_1d	$F\bar{4}d2$	$F\bar{4}d2$ $d2_1$
123	D_{4h}^1	$P4/mmm$	$P4/m\ 2/m\ 2/m$ $2_1/g$	$C4/mmm$	$C4/mmm$ nb
124	D_{4h}^2	$P4/mcc$	$P4/m\ 2/c\ 2/c$ $2_1/n$	$C4/mcc$	$C4/mcc$ nn
125	D_{4h}^3	$P4/nbm$	$P4/n\ 2/b\ 2/m$ $2_1/g$	$C4/amg_1$	$C4/amg_1$ bb
126	D_{4h}^4	$P4/nnc$	$P4/n\ 2/n\ 2/c$ $2_1/n$	$C4/acg_2$	$C4/acg_2$ bn
127	D_{4h}^5	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$ $2_1/g$	$C4/mmg_1$	$C4/mmg_1$ nb
128	D_{4h}^6	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$ $2_1/n$	$C4/mcg_2$	$C4/mcg_2$ nn
129	D_{4h}^7	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$ $2_1/g$	$C4/amm$	$C4amm$ bb
130	D_{4h}^8	$P4/ncc$	$P4/n\ 2_1/c\ 2/c$ $2_1/n$	$C4/acc$	$C4/acc$ bn
131	D_{4h}^9	$P4_2/mmc$	$P4_2/m2/m\ 2/c$ $2_1/n$	$C4_2/mcm$	$C4_2/mcm$ nn
132	D_{4h}^{10}	$P4_2/mcm$	$P4_2/m2/c\ 2/m$ $2_1/g$	$C4_2/mmc$	$C4_2/mmc$ nb
133	D_{4h}^{11}	$P4_2/nbc$	$P4_2/n2/b\ 2/c$ $2_1/n$	$C4_2/acg_1$	$C4_2/acg_1$ bn
134	D_{4h}^{12}	$P4_2/nnm$	$P4_2/n2/n\ 2/m$ $2_1/g$	$C4_2/amg_2$	$C4_2/amg_2$ bb
135	D_{4h}^{13}	$P4_2/mbc$	$P4_2/m2_1/b\ 2/c$ $2_1/n$	$C4_2/mcg_1$	$C4_2/mcg_1$ nn
136	D_{4h}^{14}	$P4_2/mnm$	$P4_2/m2_1/n\ 2/m$ $2_1/g$	$C4_2/mmg_2$	$C4_2/mmg_2$ nb
137	D_{4h}^{15}	$P4_2/nmc$	$P4_2/n\ 2_1/m\ 2/c$ $2_1/n$	$C4_2/acm$	$C4_2/acm$ bn
138	D_{4h}^{16}	$P4_2/ncm$	$P4_2/n\ 2_1/c\ 2/m$ $2_1/g$	$C4_2/amc$	$C4_2/amc$ bb
139	D_{4h}^{17}	$I4/mmm$	$I4/m\ 2/m\ 2/m$ $4_2/n\ 2_1/n\ 2_1/e$	$F4/mmm$	$F4/mmm$ $4_2/aeg_2$
140	D_{4h}^{18}	$I4/mcm$	$I4/m\ 2/c\ 2/e$ $4_2/n\ 2_1/b\ 2_1/m$	$F4/mmc$	$F4/mec$ $4_2/amg_1$
141	D_{4h}^{19}	$I4_1/amd$	$I4_1/a\ 2/m\ 2/d$ $4_3/b\ 2_1/n\ 2_1/d$	$F4_1/ddm$	$F4_1/ddm$ $4_3/ddg_2$
142	D_{4h}^{20}	$I4_1/acd$	$I4_1/a\ 2/c\ 2/d$ $4_3/b\ 2_1/b\ 2_1/d$	$F4_1/ddc$	$F4_1/ddc$ $4_3/ddg_1$

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 $g_2(\frac{1}{4},\frac{1}{4},\frac{1}{2})$. For the glide plane symbol 'e', see the *Foreword to the Fourth Edition* (*IT* 1995) and Section 1.3.2, Note (x).

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

TRIGONAL SYSTEM

No. of space group	Schoen-flies 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	Schoen-flies 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 $\bar{\mathbf{c}}$**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	$I4_132$		$I4_132$ $4_3\ 2_1$

CUBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols		
		Short	Full	Extended†
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 $\bar{\mathbf{c}}\mathbf{b}\bar{\mathbf{a}}$ 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 $\begin{array}{c} I2\ 2\ 2 \\ 2_12_12_1 \end{array}$; 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.

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: $P2_122$ ($P222_1$); *Pmm*2; $P2_1ma$ ($Pmc2_1$); *Pm*2*a* (*Pma*2).

From the standard full symbol of an *I* group of class *mmm*, the *t* subgroup of class 222 is read directly. It is either *I*222 [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 *mm*2.

Example

Ibam (72) has the following three maximal *t* subgroups of *ccn*
class *mm*2: *Iba*2; $Ib2_1m$ (*Ima*2); $I2_1am$ (*Ima*2).

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 *C*222 (for all other cases). For the three maximal *t* subgroups of class *mm*2, the two-line symbols are used.

Example

Cmce (64) has the following three maximal *t* subgroups of *bna*
class *mm*2: $Cmc2_1$; *Cm*2*e* (*Aem*2); *C*2*ce* (*Aea*2).

Finally, *Fmmm* (69) has maximal *t* subgroups *F*222 and *Fmm*2 (plus permutations), whereas *Fddd* (70) has *F*222 and *Fdd*2 (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 *C*211 (*C*2), *C*121 (*C*2) and $C112_1$. The last one reduces to $P112_1$ ($P2_1$).
(2) *Ama*2 (40) has the maximal *t* subgroups *Am*11, reducible to *Pm*, *A*1*a*1 (*Cc*) and *A*112 (*C*2).
(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), 4*m*(*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 4*mm*, $\bar{4}2m$ 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 **a**, **b**, **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.

(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 $\begin{array}{c}C4_p2\;2\\ 2_1\end{array}$, 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 $\begin{array}{c}C\bar{4}2\;c\\ 2_1\end{array}$, 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 $\begin{array}{c}C4_2cm\\ n\end{array}$, 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 $\begin{array}{c}C4_2/mmc\\ n\;b\end{array}$, 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 $\begin{array}{c}C4/amg_1\\ bb\end{array}$ 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 $\begin{array}{c}I4\;ce\\ 4_2bm\end{array}$. 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 $\begin{array}{c}I4/m\;ce\\ 4_2/nbm\end{array}$. One obtains the subgroups of example (1) with an additional *m* or *n* plane perpendicular to **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 $\begin{array}{c}I4/m2/c\;2/e\\ 4_2/n2_1/b2_1/m\end{array}$ 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].

Examples

(1) $P4_2/mbc$ (135). From the full symbol, the *first* maximal t subgroup is found to be $P2_1/b\,2_1/a\,2/m$ ($Pbam$). The C-cell symbol is $C4_2/m\,cg_1$ and gives rise to the *second* maximal orthorhombic t subgroup $Cccm$, cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$.

(2) $I4/m\,cm$ (140). Similarly, the *first* orthorhombic maximal t subgroup is $Iccm$ ($Ibam$); the *second* maximal orthorhombic t subgroup is obtained from the F-cell symbol as $F\begin{smallmatrix} ban \\ c\,c\,m \\ mmn \end{smallmatrix}$ ($Fmmm$), cell $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$.

These examples show that P- and C-cell, as well as I- and F-cell descriptions of tetragonal groups have to be considered together.

(iii) *Monoclinic subgroups*

Only space groups of classes 4, $\bar{4}$ and $4/m$ have maximal monoclinic t subgroups.

Examples

(1) $P4_1$ (76) has the subgroup $P112_1$ ($P2_1$). The C-cell description does not add new features: $C112_1$ is reducible to $P2_1$.

(2) $I4_1/a$ (88) has the subgroup $I112_1/a$, equivalent to $I112/a$ ($C2/c$). The F-cell description yields the same subgroup $F11\,2/d$, again reducible to $C2/c$.

4.3.5. Trigonal and hexagonal systems

The trigonal and hexagonal crystal systems are considered together, because they form the hexagonal 'crystal family', as explained in Chapter 2.1. Hexagonal lattices occur in both systems, whereas rhombohedral lattices occur only in the trigonal system.

4.3.5.1. *Historical note*

The 1935 edition of *International Tables* contains the symbols C and H for the *hexagonal lattice* and R for the *rhombohedral lattice.* C recalls that the hexagonal lattice can be described by a double rectangular C-centred cell (orthohexagonal axes); H was used for a hexagonal triple cell (see below); R designates the rhombohedral lattice and is used for both the rhombohedral description (primitive cell) and the hexagonal description (triple cell).

In the 1952 edition the following changes took place (*cf.* pages x, 51 and 544 of *IT* 1952): The lattice symbol C was replaced by P for reasons of consistency; the H description was dropped. The symbol R was kept for both descriptions, rhombohedral and hexagonal. The tertiary symmetry element in the short Hermann–Mauguin symbols of class 622, which was omitted in *IT* (1935), was re-established.

In the present volume, the use of P and R is the same as in *IT* (1952). The H cell, however, reappears in the sub- and supergroup data of Part 7 and in Table 4.3.2.1 of this section, where short symbols for the H description of trigonal and hexagonal space groups are given. The C cell reappears in the subgroup data for all trigonal and hexagonal space groups having symmetry elements orthogonal to the main axis.

4.3.5.2. *Primitive cells*

The primitive cells of the hexagonal and the rhombohedral lattice, hP and hR, are defined in Table 2.1.2.1 In Part 7, the 'rhombohedral' description of the hR lattice is designated by 'rhombohedral axes'; *cf.* Chapter 1.2.

4.3.5.3. *Multiple cells*

Multiple cells are frequently used to describe both the hexagonal and the rhombohedral lattice.

(i) *The triple hexagonal R cell; cf. Chapters 1.2 and 2.1*

When the lattice is *rhombohedral hR* (primitive cell $\mathbf{a}, \mathbf{b}, \mathbf{c}$), the triple R cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ corresponds to the 'hexagonal description' of the rhombohedral lattice. There are three right-handed *obverse R* cells:

$$\begin{aligned} R_1: &\quad \mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{b} - \mathbf{c}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}; \\ R_2: &\quad \mathbf{a}' = \mathbf{b} - \mathbf{c}; \quad \mathbf{b}' = \mathbf{c} - \mathbf{a}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}; \\ R_3: &\quad \mathbf{a}' = \mathbf{c} - \mathbf{a}; \quad \mathbf{b}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}. \end{aligned}$$

Three further right-handed R cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a 180° rotation around $\mathbf{c}'$. These cells are *reverse*. The transformations between the triple R cells and the primitive rhombohedral cell are given in Table 5.1.3.1 and Fig. 5.1.3.6.

The obverse triple R cell has 'centring points' at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3},$$

whereas the reverse R cell has 'centring points' at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{2}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{1}{3},\tfrac{2}{3}.$$

In the space-group tables of Part 7, the obverse R_1 cell is used, as illustrated in Fig. 2.2.6.9. This 'hexagonal description' is designated by 'hexagonal axes'.

(ii) *The triple rhombohedral D cell*

Parallel to the 'hexagonal description of the rhombohedral lattice' there exists a 'rhombohedral description of the hexagonal lattice'. Six right-handed rhombohedral cells (here denoted by D) with cell vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ of equal lengths are obtained from the hexagonal P cell $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ by the following transformations and by cyclic permutations of $\mathbf{a}', \mathbf{b}', \mathbf{c}'$:

$$\begin{aligned} D_1: &\quad \mathbf{a}' = \mathbf{a} + \mathbf{c}; \quad \mathbf{b}' = \mathbf{b} + \mathbf{c}; \quad \mathbf{c}' = -(\mathbf{a} + \mathbf{b}) + \mathbf{c} \\ D_2: &\quad \mathbf{a}' = -\mathbf{a} + \mathbf{c}; \quad \mathbf{b}' = -\mathbf{b} + \mathbf{c}; \quad \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}. \end{aligned}$$

The transformation matrices are listed in Table 5.1.3.1. D_2 follows from D_1 by a 180° rotation around [111]. The D cells are triple rhombohedral cells with 'centring' points at

$$0,0,0; \quad \tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{3}; \quad \tfrac{2}{3},\tfrac{2}{3},\tfrac{2}{3}.$$

The D cell, not used in practice and not considered explicitly in the present volume, is useful for a deeper understanding of the relations between hexagonal and rhombohedral lattices.

(iii) *The triple hexagonal H cell; cf. Chapter 1.2*

Generally, a hexagonal lattice hP is described by means of the smallest hexagonal P cell. An alternative description employs a larger hexagonal H-centred cell of three times the volume of the P cell; this cell was extensively used in *IT* (1935), see *Historical note* above.

There are three right-handed orientations of the H cell (basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$) with respect to the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the P cell:

$$\begin{aligned} H_1: &\quad \mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{a} + 2\mathbf{b}; \quad \mathbf{c}' = \mathbf{c} \\ H_2: &\quad \mathbf{a}' = 2\mathbf{a} + \mathbf{b}; \quad \mathbf{b}' = -\mathbf{a} + \mathbf{b}; \quad \mathbf{c}' = \mathbf{c} \\ H_3: &\quad \mathbf{a}' = \mathbf{a} + 2\mathbf{b}; \quad \mathbf{b}' = -2\mathbf{a} - \mathbf{b}; \quad \mathbf{c}' = \mathbf{c}. \end{aligned}$$

The transformations are given in Table 5.1.3.1 and Fig. 5.1.3.8. The new vectors $\mathbf{a}'$ and $\mathbf{b}'$ are rotated in the ab plane by $-30°(H_1)$, $+30°(H_2)$, $+90°(H_3)$ with respect to the old vectors $\mathbf{a}$ and $\mathbf{b}$. Three further right-handed H cells are obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$, *i.e.* by a rotation of 180° around $\mathbf{c}'$.

The H cell has 'centring' points at

$$0,0,0; \quad \tfrac{2}{3},\tfrac{1}{3},0; \quad \tfrac{1}{3},\tfrac{2}{3},0.$$

Secondary and tertiary symmetry elements of the *P* cell are interchanged in the *H* cell, and the general position in the *H* cell is easily obtained, as illustrated by the following example.

Example

The space-group symbol *P*3*m*1 in the *P* cell **a**, **b**, **c** becomes *H*31*m* in the *H* cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. To obtain the general position of *H*31*m*, consider the coordinate triplets of *P*31*m* and add the centring translations $0, 0, 0;\ \frac{2}{3}, \frac{1}{3}, 0;\ \frac{1}{3}, \frac{2}{3}, 0$.

(iv) *The double orthohexagonal C cell*

The *C*-centred cell which is defined by the so-called 'orthohexagonal' vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ has twice the volume of the *P* cell. There are six right-handed orientations of the *C* cell, which are C_1, C_2 and C_3 plus three further ones obtained by changing $\mathbf{a}'$ and $\mathbf{b}'$ to $-\mathbf{a}'$ and $-\mathbf{b}'$:

$$\begin{aligned} C_1 &: \mathbf{a}' = \mathbf{a}\quad; & \mathbf{b}' &= \mathbf{a} + 2\mathbf{b}; & \mathbf{c}' &= \mathbf{c}\\ C_2 &: \mathbf{a}' = \mathbf{a} + \mathbf{b}; & \mathbf{b}' &= -\mathbf{a} + \mathbf{b}; & \mathbf{c}' &= \mathbf{c}\\ C_3 &: \mathbf{a}' = \mathbf{b}; & \mathbf{b}' &= -2\mathbf{a} - \mathbf{b}; & \mathbf{c}' &= \mathbf{c}. \end{aligned}$$

Transformation matrices are given in Table 5.1.3.1 and illustrations in Fig. 5.1.3.7. Here $\mathbf{b}'$ is the long axis.

4.3.5.4. *Relations between symmetry elements*

In the hexagonal crystal classes 62(2), 6*m*(*m*) and $\bar{6}2(m)$ or $\bar{6}m(2)$, where the tertiary symmetry element is between parentheses, the following products hold:

$$6 \times 2 = (2) = \bar{6} \times m; \quad 6 \times m = (m) = \bar{6} \times 2$$

or

$$6 \times 2 \times (2) = 6 \times m \times (m) = \bar{6} \times 2 \times (m) = \bar{6} \times m \times (2) = 1.$$

The same relations hold for the corresponding Hermann–Mauguin space-group symbols.

4.3.5.5. *Additional symmetry elements*

Parallel axes 2 and 2_1 occur perpendicular to the principal symmetry axis. Examples are space groups *R*32 (155), *P*321 (150) and *P*312 (149), where the screw components are $\frac{1}{2}, \frac{1}{2}, 0$ (rhombohedral axes) or $\frac{1}{2}, 0, 0$ (hexagonal axes) for *R*32; $\frac{1}{2}, 0, 0$ for *P*321; and $\frac{1}{2}, 1, 0$ for *P*312. Hexagonal examples are *P*622 (177) and $P\bar{6}2c$ (190).

Likewise, mirror planes *m* parallel to the main symmetry axis alternate with glide planes, the glide components being perpendicular to the principal axis. Examples are *P*3*m*1 (156), *P*31*m* (157), *R*3*m* (160) and *P*6*mm* (183).

Glide planes *c* parallel to the main axis are interleaved by glide planes *n*. Examples are *P*3*c*1 (158), *P*31*c* (159), *R*3*c* (161, hexagonal axes), $P\bar{6}c2$ (188). In *R*3*c* and $R\bar{3}c$, the glide component $0, 0, \frac{1}{2}$ for hexagonal axes becomes $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ for rhombohedral axes, *i.e.* the *c* glide changes to an *n* glide. Thus, if the space group is referred to rhombohedral axes, diagonal *n* planes alternate with diagonal *a*, *b* or *c* planes (*cf.* Section 1.4.4).

In *R* space groups, all additional symmetry elements with glide and screw components have their origin in the action of an integral lattice translation. This is also true for the axes 3_1 and 3_2 which appear in all *R* space groups (*cf.* Table 4.1.2.2). For this reason, the 'rhombohedral centring' *R* is not included in Table 4.1.2.3, which contains only the centrings *A*, *B*, *C*, *I*, *F*.

4.3.5.6. *Group–subgroup relations*

4.3.5.6.1. *Maximal k subgroups*

Maximal *k* subgroups of index [3] are obtained by 'decentring' the triple cells *R* (hexagonal description), *D* and *H* in the trigonal system, *H* in the hexagonal system. Any one of the three centring points may be taken as origin of the subgroup.

(i) *Trigonal system*

Examples

(1) *P*3*m*1 (156) (cell **a**, **b**, **c**) is equivalent to *H*31*m* ($\mathbf{a}'$, $\mathbf{b}'$, **c**). Decentring of the *H* cell yields maximal non-isomorphic *k* subgroups of type *P*31*m*. Similarly, *P*31*m* (157) has maximal subgroups of type *P*3*m*1; thus, one can construct infinite chains of subgroup relations of index [3], tripling the cell at each step:

$$P3m1 \rightarrow P31m \rightarrow P3m1 \ldots$$

(2) *R*3 (146), by decentring the triple hexagonal *R* cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$, yields the subgroups *P*3, $P3_1$ and $P3_2$ of index [3].

(3) Likewise, decentring of the triple rhombohedral cells D_1 and D_2 gives rise, for each cell, to the rhombohedral subgroups of a trigonal *P* group, again of index [3].

Combining (2) and (3), one may construct infinite chains of subgroup relations, tripling the cell at each step:

$$P3 \rightarrow R3 \rightarrow P3 \rightarrow R3 \ldots$$

These chains illustrate best the connections between rhombohedral and hexagonal lattices.

(4) Special care must be applied when secondary or tertiary symmetry elements are present. Combining (1), (2) and (3), one has for instance:

$$P31c \rightarrow R3c \rightarrow P3c1 \rightarrow P31c \rightarrow R3c \ldots$$

(5) Rhombohedral subgroups, found by decentring the triple cells D_1 and D_2, are given under block **IIb** and are referred there to hexagonal axes, $\mathbf{a}', \mathbf{b}', \mathbf{c}$ as listed below. Examples are space groups *P*3 (143) and $P\bar{3}1c$ (163)

$$\begin{aligned} \mathbf{a}' &= \mathbf{a} - \mathbf{b}, & \mathbf{b}' &= \mathbf{a} + 2\mathbf{b}, & \mathbf{c}' &= 3\mathbf{c};\\ \mathbf{a}' &= 2\mathbf{a} + \mathbf{b}, & \mathbf{b}' &= -\mathbf{a} + \mathbf{b}, & \mathbf{c}' &= 3\mathbf{c}. \end{aligned}$$

(ii) *Hexagonal system*

Examples

(1) $P\bar{6}2c$ (190) is described as $H\bar{6}c2$ in the triple cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$; decentring yields the non-isomorphic subgroup $P\bar{6}c2$.

(2) *P*6/*mcc* (192) (cell **a**, **b**, **c**) keeps the same symbol in the *H* cell and, consequently, gives rise to the maximal isomorphic subgroup *P*6/*mcc* with cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. An analogous result applies whenever secondary and tertiary symmetry elements in the Hermann–Mauguin symbol are the same and also to space groups of classes 6, $\bar{6}$ and 6/*m*.

4.3.5.6.2. *Maximal t subgroups*

Maximal *t* subgroups of index [2] are read directly from the full symbol of the space groups of classes 32, 3*m*, $\bar{3}m$, 622, 6*mm*, $\bar{6}2m$, 6/*mmm*.

Maximal *t* subgroups of index [3] follow from the third power of the main-axis operation. Here the *C*-cell description is valuable.

(i) *Trigonal system*

(*a*) *Trigonal subgroups*

Examples

(1) $R\bar{3}2/c$ (167) has *R*3*c*, *R*32 and $R\bar{3}$ as maximal *t* subgroups of index [2].

(2) $P\bar{3}c1$ (165) has *P*3*c*1, *P*321 and $P\bar{3}$ as maximal *t* subgroups of index [2].

(*b*) *Orthorhombic subgroups*

No orthorhombic subgroups of trigonal space groups exist, in spite of the existence of an orthohexagonal *C* cell.

(*c*) *Monoclinic subgroups*

All trigonal space groups with secondary or tertiary symmetry elements have monoclinic *C*-centred maximal *t* subgroups of index [3].

Example

$P\bar{3}1c$ (163), $P\bar{3}c1$ (165) and $R\bar{3}c$ (167) have subgroups of type $C2/c$.

(*d*) *Triclinic subgroups*

All trigonal space groups without secondary or tertiary symmetry elements have triclinic maximal *t* subgroups of index [3].

Example

$P\bar{3}$ (147) and $R\bar{3}$ (148) have subgroups $P\bar{1}$.

(ii) *Hexagonal system*

(*a*) *Hexagonal subgroups*

Example

$P6_3/m\,2/c\,2/m$ (193) has maximal *t* subgroups $P6_3/m$, $P6_322$, $P6_3cm$, $P\bar{6}2m$ and $P\bar{6}c2$ of index [2].

(*b*) *Trigonal subgroups*

The second and fourth powers of sixfold operations are threefold operations; thus, all hexagonal space groups have maximal trigonal *t* subgroups of index [2]. In space groups of classes 622, $6mm$, $\bar{6}2m$, $6/mmm$ with secondary and tertiary symmetry elements, trigonal *t* subgroups always occur in pairs.

Examples

(1) $P6_1$ (169) contains $P3_1$ of index [2].
(2) $P\bar{6}2c$ (190) has maximal *t* subgroups $P321$ and $P31c$; $P6_122$ (178) has subgroups $P3_121$ and $P3_112$, all of index [2].
(3) $P6_3/mcm$ (193) contains the operation $\bar{3}$ $[=(6_3)^2 \times \bar{1}]$ and thus has maximal *t* subgroups $P\bar{3}c1$ and $P\bar{3}1m$ of index [2].

(*c*) *Orthorhombic and monoclinic subgroups*

The third power of the sixfold operation is a twofold operation: accordingly, maximal orthorhombic *t* subgroups of index [3] are derived from the *C*-cell description of space groups of classes 622, $6mm$, $\bar{6}2m$ and $6/mmm$. Monoclinic *P* subgroups of index [3] occur in crystal classes 6, $\bar{6}$ and $6/m$.

Examples

(1) $P\bar{6}2c$ (190) becomes $C\bar{6}2c$ in the *C* cell; with $(\bar{6})^3 = m$, one obtains $C2cm$ (sequence **a**, **b**, **c**) as a maximal *t* subgroup of index [3]. The standard symbol is $Ama2$.
(2) $P6_3/mcm$ (193) has maximal orthorhombic *t* subgroups of type $Cmcm$ of index [3]. With the examples under (*a*) and (*b*), this exhausts all maximal *t* subgroups of $P6_3/mcm$.
(3) $P6_1$ (169) has a maximal *t* subgroup $P2_1$; $P6_3/m$ (176) has $P2_1/m$ as a maximal *t* subgroup.

4.3.6. Cubic system

4.3.6.1. *Historical note and arrangement of tables*

In the synoptic tables of *IT* (1935) and *IT* (1952), for cubic space groups short and full Hermann–Mauguin symbols were listed. They agree, except that in *IT* (1935) the tertiary symmetry element of the space groups of class 432 was omitted; it was re-established in *IT* (1952).

In the present edition, the symbols of *IT* (1952) are retained, with one exception. In the space groups of crystal classes $m\bar{3}$ and $m\bar{3}m$, the short symbols contain $\bar{3}$ instead of 3 (*cf.* Section 2.2.4). In Table 4.3.2.1, short and full symbols for all cubic space groups are given. In addition, for centred groups *F* and *I* and for *P* groups with tertiary symmetry elements, extended space-group symbols are listed. In space groups of classes 432 and $\bar{4}3m$, the product rule (as defined below) is applied in the first line of the extended symbol.

4.3.6.2. *Relations between symmetry elements*

Conventionally, the representative directions of the primary, secondary and tertiary symmetry elements are chosen as [001], [111], and [1$\bar{1}$0] (*cf.* Table 2.2.4.1 for the equivalent directions). As in tetragonal and hexagonal space groups, tertiary symmetry elements are not independent. In classes 432, $\bar{4}3m$ and $m\bar{3}m$, there are product rules

$$4 \times 3 = (2); \quad \bar{4} \times 3 = (m) = 4 \times \bar{3},$$

where the tertiary symmetry element is in parentheses; analogous rules hold for the space groups belonging to these classes. When the symmetry directions of the primary and secondary symmetry elements are chosen along [001] and [111], respectively, the tertiary symmetry direction is [011], according to the product rule. In order to have the tertiary symmetry direction along [1$\bar{1}$0], one has to choose the somewhat awkward primary and secondary symmetry directions [010] and [$\bar{1}$1$\bar{1}$].

Examples

(1) In $P\bar{4}3n$ (218), with the choice of the 3 axis along [$\bar{1}$1$\bar{1}$] and of the $\bar{4}$ axis parallel to [010], one finds $\bar{4} \times 3 = n$, the *n* glide plane being in x, x, z, as shown in the space-group diagram.
(2) In $F\bar{4}3c$ (219), one has the same product rule as above; the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$, however, associates with the *n* glide plane a *c* glide plane, also located in x, x, z (*cf.* Table 4.1.2.3). In the space-group diagram and symbol, *c* was preferred to *n*.

4.3.6.3. *Additional symmetry elements*

Owing to periodicity, the tertiary symmetry elements alternate; diagonal axes 2 alternate with parallel screw axes 2_1; diagonal planes *m* alternate with parallel glide planes *g*; diagonal *n* planes, *i.e.* planes with glide components $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, alternate with glide planes *a*, *b* or *c* (*cf.* Chapter 4.1 and Tables 4.1.2.2 and 4.1.2.3). For the meaning of the various glide planes *g*, see Section 11.1.2 and the entries *Symmetry operations* in Part 7.

4.3.6.4. *Group–subgroup relations*

4.3.6.4.1. *Maximal k subgroups*

The extended symbol of $Fm\bar{3}$ (202) shows clearly that $Pm\bar{3}$, $Pn\bar{3}$, $Pb\bar{3}$ ($Pa\bar{3}$) and $Pa\bar{3}$ are maximal subgroups. $Pm\bar{3}m$, $Pn\bar{3}n$, $Pm\bar{3}n$ and $Pn\bar{3}m$ are maximal subgroups of $Im\bar{3}m$ (229). Space groups with *d* glide planes have no *k* subgroup of lattice *P*.

4.3.6.4.2. *Maximal t subgroups*

(*a*) *Cubic subgroups*

The cubic space groups of classes $m\bar{3}$, 432 and $\bar{4}3m$ have maximal cubic subgroups of class 23 which are found by simple inspection of the full symbol.

Examples

$Ia\bar{3}$ (206), full symbol $I2_1/a\bar{3}$, contains $I2_13$. $P2_13$ is a maximal subgroup of $P4_132$ (213) and its enantiomorph $P4_332$ (212). A more difficult example is $I\bar{4}3d$ (220) which contains $I2_13$.*

The cubic space groups of class $m\bar{3}m$ have maximal subgroups which belong to classes 432 and $\bar{4}3m$.

Examples

$F4/m\bar{3}2/c$ (226) contains $F432$ *and* $F\bar{4}3c$; $I4_1/a\bar{3}2/d$ (230) contains $I4_132$ *and* $I\bar{4}3d$.

(*b*) *Tetragonal subgroups*

In the cubic space groups of classes 432 and $\bar{4}3m$, the primary and tertiary symmetry elements are relevant for deriving maximal tetragonal subgroups.

Examples

The groups $P432$ (207), $P4_232$ (208), $P4_332$ (212) and $P4_132$ (213) have maximal tetragonal *t* subgroups of index [3]: $P422$, $P4_222, P4_32_12$ and $P4_12_12$. $I432$ (211) gives rise to $I422$ with the same cell. $F432$ (209) also gives rise to $I422$, but *via* $F422$, so that the final unit cell is $a\sqrt{2}/2, a\sqrt{2}/2, a$.

In complete analogy, the groups $P\bar{4}3m$ (215) and $P\bar{4}3n$ (218) have maximal subgroups $P\bar{4}2m$ and $P\bar{4}2c$.†

For the space groups of class $m\bar{3}m$, the full symbols are needed to recognize their tetragonal maximal subgroups of class $4/mmm$. The primary symmetry planes of the cubic space group are conserved in the primary *and* secondary symmetry elements of the tetragonal subgroup: *m*, *n* and *d* remain in the tetragonal symbol; *a* remains *a* in the primary and becomes *c* in the secondary symmetry element of the tetragonal symbol.

Example

$P4_2/n\,\bar{3}\,2/m$ (224) and $I4_1/a\,\bar{3}\,2/d$ (230) have maximal subgroups $P4_2/n\,2/n\,2/m$ and $I4_1/a\,2/c\,2/d$, respectively, $F4_1/d\,\bar{3}\,2/c$ (228) gives rise to $F4_1/d\,2/d\,2/c$, which is equivalent to $I4_1/a\,2/c\,2/d$, all of index [3].

(*c*) *Rhombohedral subgroups*‡

Here the secondary and tertiary symmetry elements of the cubic space-group symbols are relevant. For space groups of classes 23, $m\bar{3}$, 432, the maximal *R* subgroups are $R3$, $R\bar{3}$ and $R32$, respectively. For space groups of class $\bar{4}3m$, the maximal *R* subgroup is $R3m$ when the tertiary symmetry element is *m* and $R3c$ otherwise. Finally, for space groups of class $m\bar{3}m$, the maximal *R* subgroup is $R\bar{3}m$ when the tertiary symmetry element is *m* and $R\bar{3}c$ otherwise. All subgroups are of index [4].

(*d*) *Orthorhombic subgroups*

Maximal orthorhombic space groups of index [3] are easily derived from the cubic space-group symbols of classes 23 and $m\bar{3}$.‡ Thus, $P23$, $F23$, $I23$, $P2_13$, $I2_13$ (195–199) have maximal subgroups $P222$, $F222$, $I222$, $P2_12_12_1$, $I2_12_12_1$, respectively. Likewise, maximal subgroups of $Pm\bar{3}$, $Pn\bar{3}$, $Fm\bar{3}$, $Fd\bar{3}$, $Im\bar{3}$, $Pa\bar{3}$, $Ia\bar{3}$ (200–206) are *Pmmm*, *Pnnn*, *Fmmm*, *Fddd*, *Immm*, *Pbca*, *Ibca*, respectively. The lattice type (*P*, *F*, *I*) is conserved and only the primary symmetry element has to be considered.

* From the product rule it follows that $\bar{4}$ and *d* have the same translation component so that $(\bar{4})^2 = 2_1$.

† The tertiary cubic symmetry element *n* becomes *c* in tetragonal notation.

‡ They have already been given in *IT* (1935).

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4.1

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