

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 \underline{abc} and \bar{cba}), 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 \underline{abc} , 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 \bar{cba} .

(ii) Unique axis c

In the third column, headed by \underline{abc} , 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 \bar{bac} .

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 \underline{abc} contains the three symbols $C1 2/c 1$, $A1 2/n 1$ 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 \bar{cba} 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 \underline{abc} 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 \bar{bac} 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:

\underline{abc}	\bar{cba}	cab	$ac\bar{b}$	bca	\bar{bac}	Unique axis b
bca	\bar{acb}	$ab\underline{c}$	$ba\bar{c}$	cab	\bar{cba}	Unique axis c
cab	\bar{bac}	bca	$cb\bar{a}$	\underline{abc}	\bar{acb}	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 \bar{cab} , first line, third column. Compared to the initial setting \underline{abc} , it contains the ‘unique axis b ’ in the third place and, consequently, must be identified with the setting \underline{abc} , 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 \bar{bac} in the first line, sixth column. It contains the ‘unique axis b ’ in the first place and thus must be identified with the setting \bar{acb} , 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

4.3. SYMBOLS FOR SPACE GROUPS

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	$P\bar{1}$
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						Unique axis b Unique axis c Unique axis a
			$\underline{\text{abc}}$	$\underline{\text{cba}}$	$\underline{\text{abc}}$	$\underline{\text{bac}}$	$\underline{\text{abc}}$	$\underline{\text{acb}}$	
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 $I121$ 2_1	$A121$ 2_1 $C121$ 2_1 $I121$ 2_1	$A112$ 2_1 $B112$ 2_1 $I112$ 2_1	$B112$ 2_1 $A112$ 2_1 $I112$ 2_1	$B211$ 2_1 $C211$ 2_1 $I211$ 2_1	$C211$ 2_1 $B211$ 2_1 $I211$ 2_1	Cell choice 1 Cell choice 2 Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$ $P1n1$ $P1a1$	$P1a1$ $P1n1$ $P1c1$	$P11a$ $P11n$ $P11b$	$P11b$ $P11n$ $P11a$	$Pb11$ $Pn11$ $Pc11$	$Pc11$ $Pn11$ $Pb11$	Cell choice 1 Cell choice 2 Cell choice 3
8	C_s^3	Cm	$C1m1$ a $A1m1$ c $I1m1$ n	$A1m1$ c $C1m1$ a $I1m1$ n	$A11m$ b $B11m$ a $I11m$ n	$B11m$ a $A11m$ b $I11m$ n	$Bm11$ b $Cm11$ b $Im11$ n	$Cm11$ b $Bm11$ c $Im11$ n	Cell choice 1 Cell choice 2 Cell choice 3
9	C_s^4	Cc	$C1c1$ n $A1n1$ a $I1a1$ c	$A1a1$ n $C1n1$ c $I1c1$ a	$A11a$ n $B11n$ b $I11b$ a	$B11b$ n $A11n$ a $I11a$ b	$Bb11$ n $Cn11$ c $Ic11$ b	$Cc11$ n $Bn11$ b $Ib11$ c	Cell choice 1 Cell choice 2 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	$C2/m$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$ $A1\frac{2}{m}1$ $\frac{2_1}{c}$ $I1\frac{2}{m}1$ $\frac{2_1}{n}$	$A1\frac{2}{m}1$ $\frac{2_1}{c}$ $C1\frac{2}{m}1$ $\frac{2_1}{a}$ $I1\frac{2}{m}1$ $\frac{2_1}{n}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$ $B11\frac{2}{m}$ $\frac{2_1}{a}$ $I11\frac{2}{m}$ $\frac{2_1}{n}$	$B11\frac{2}{m}$ $\frac{2_1}{a}$ $A11\frac{2}{m}$ $\frac{2_1}{b}$ $I11\frac{2}{m}$ $\frac{2_1}{n}$	$B\frac{2}{m}11$ $\frac{2_1}{c}$ $C\frac{2}{m}11$ $\frac{2_1}{b}$ $I\frac{2}{m}11$ $\frac{2_1}{n}$	$C\frac{2}{m}11$ $\frac{2_1}{b}$ $B\frac{2}{m}11$ $\frac{2_1}{c}$ $I\frac{2}{m}11$ $\frac{2_1}{n}$	Cell choice 1 Cell choice 2 Cell choice 3
13	C_{2h}^4	$P2/c$	$P1\frac{2}{c}1$ $P1\frac{2}{n}1$ $P1\frac{2}{a}1$	$P1\frac{2}{a}1$ $P1\frac{2}{n}1$ $P1\frac{2}{c}1$	$P11\frac{2}{a}$ $P11\frac{2}{n}$ $P11\frac{2}{b}$	$P11\frac{2}{b}$ $P11\frac{2}{n}$ $P11\frac{2}{a}$	$P\frac{2}{b}11$ $P\frac{2}{n}11$ $P\frac{2}{c}11$	$P\frac{2}{c}11$ $P\frac{2}{n}11$ $P\frac{2}{b}11$	Cell choice 1 Cell choice 2 Cell choice 3

4. SYNOPTIC TABLES OF SPACE-GROUP SYMBOLS

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						Unique axis <i>b</i>	Unique axis <i>c</i>	Unique axis <i>a</i>
			abc	c̄ba	abc̄	bāc	abc̄	ācb			
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	Cell choice 2	Cell choice 3
			$P1\frac{2_1}{n}1$	$P1\frac{2_1}{n}1$	$P11\frac{2_1}{n}$	$P11\frac{2_1}{a}$	$P\frac{2_1}{n}11$	$P\frac{2_1}{n}11$			
			$P1\frac{2_1}{a}1$	$P1\frac{2_1}{c}1$	$P11\frac{2_1}{b}$	$P11\frac{2_1}{a}$	$P\frac{2_1}{c}11$	$P\frac{2_1}{b}11$			
15	C_{2h}^6	$C2/c$	$C1\frac{2}{c}1$	$A1\frac{2}{a}1$	$A11\frac{2}{a}$	$B11\frac{2}{b}$	$B\frac{2}{b}11$	$C\frac{2}{c}11$	Cell choice 1	Cell choice 2	Cell choice 3
			$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$			
			$A1\frac{2}{n}1$	$C1\frac{2}{n}1$	$B11\frac{2}{n}$	$A11\frac{2}{n}$	$C\frac{2}{n}11$	$B\frac{2}{n}11$			
			$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$			
			$I1\frac{2}{a}1$	$I1\frac{2}{c}1$	$I11\frac{2}{b}$	$I11\frac{2}{a}$	$I\frac{2}{c}11$	$I\frac{2}{b}11$	Cell choice 3		
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$			

ORTHORHOMBIC SYSTEM

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						P222	P222	P222
			abc (standard)	bāc	cab	̄cba	bca	ācb			
16	D_2^1	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$
17	D_2^2	$P222_1$	$P222_1$	$P222_1$	$P2_122$	$P2_122$	$P2_122$	$P2_122$	$P22_12$	$P22_12$	$P22_12$
18	D_2^3	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P22_12_1$	$P22_12_1$	$P22_12_1$	$P22_12_1$	$P2_122_1$	$P2_122_1$	$P2_122_1$
19	D_2^4	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
20	D_2^5	$C222_1$	$C222_1$	$C222_1$	$A2_122$	$A2_122$	$A2_122$	$A2_122$	$B22_12$	$B22_12$	$B22_12$
21	D_2^6	$C222$	$C222$	$C222$	$A222$	$A222$	$A222$	$A222$	$B222$	$B222$	$B222$
22	D_2^7	$F222$	$F222$	$F222$	$F222$	$F222$	$F222$	$F222$	$F222$	$F222$	$F222$
23	D_2^8	$I222$	$I222$	$I222$	$I222$	$I222$	$I222$	$I222$	$I222$	$I222$	$I222$
24	D_2^9	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$
25	C_{2v}^1	$Pmm2$	$Pmm2$	$Pmm2$	$P2mm$	$P2mm$	$P2mm$	$Pm2m$	$Pm2m$	$Pm2m$	$Pm2m$
26	C_{2v}^2	$Pmc2_1$	$Pmc2_1$	$Pcm2_1$	$P2_1ma$	$P2_1am$	$P2_1am$	$Pb2_1m$	$Pb2_1m$	$Pb2_1m$	$Pb2_1m$
27	C_{2v}^3	$Pcc2$	$Pcc2$	$Pcc2$	$P2aa$	$P2aa$	$P2aa$	$Pb2b$	$Pb2b$	$Pb2b$	$Pb2b$
28	C_{2v}^4	$Pma2$	$Pma2$	$Pbm2$	$P2mb$	$P2mb$	$P2mb$	$Pc2m$	$Pc2m$	$Pc2m$	$Pc2m$
29	C_{2v}^5	$Pca2_1$	$Pca2_1$	$Pbc2_1$	$P2_1ab$	$P2_1ab$	$P2_1ab$	$Pc2_1b$	$Pc2_1b$	$Pc2_1b$	$Pc2_1b$
30	C_{2v}^6	$Pnc2$	$Pnc2$	$Pcn2$	$P2na$	$P2na$	$P2na$	$Pb2n$	$Pb2n$	$Pb2n$	$Pb2n$
31	C_{2v}^7	$Pmn2_1$	$Pmn2_1$	$Pnm2_1$	$P2_1mn$	$P2_1mn$	$P2_1mn$	$Pn2m$	$Pn2m$	$Pn2m$	$Pn2m$
32	C_{2v}^8	$Pba2$	$Pba2$	$Pba2$	$P2cb$	$P2cb$	$P2cb$	$Pc2a$	$Pc2a$	$Pc2a$	$Pc2a$
33	C_{2v}^9	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1nb$	$P2_1nb$	$Pc2_1n$	$Pc2_1n$	$Pc2_1n$	$Pc2_1n$
34	C_{2v}^{10}	$Pnn2$	$Pnn2$	$Pnn2$	$P2nn$	$P2nn$	$P2nn$	$Pn2n$	$Pn2n$	$Pn2n$	$Pn2n$

4.3. SYMBOLS FOR SPACE GROUPS

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{c}	ca b	\bar{c} ba	bca	\bar{a} c \bar{b}
35	C_{2v}^{11}	$Cmm2$	$Cmm2$ $ba2$	$Cmm2$ $ba2$	$A2mm$ $2cb$	$A2mm$ $2cb$	$Bm2m$ $c2a$	$Bm2m$ $c2a$
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}	$Ccc2$	$Ccc2$ $nn2$	$Ccc2$ $nn2$	$A2aa$ $2nn$	$A2aa$ $2nn$	$Bb2b$ $n2n$	$Bb2b$ $n2n$
38	C_{2v}^{14}	$Amm2$	$Amm2$ $nc2_1$	$Bmm2$ $cn2_1$	$B2mm$ 2_1na	$C2mm$ 2_1an	$Cm2m$ $b2_1n$	$Am2m$ $n2_1b$
39*	C_{2v}^{15}	$Aem2$	$Aem2$ $ec2_1$	$Bme2$ $ce2_1$	$B2em$ 2_1ea	$C2me$ 2_1ae	$Cm2e$ $b2_1e$	$Ae2m$ $e2_1b$
40	C_{2v}^{16}	$Ama2$	$Ama2$ $nn2_1$	$Bbm2$ $nn2_1$	$B2mb$ 2_1nn	$C2cm$ 2_1nn	$Cc2m$ $n2_1n$	$Am2a$ $n2_1n$
41*	C_{2v}^{17}	$Aea2$	$Aea2$ $en2_1$	$Bbe2$ $ne2_1$	$B2eb$ 2_1en	$C2ce$ 2_1ne	$Cc2e$ $n2_1e$	$Ae2a$ $e2_1n$
42	C_{2v}^{18}	$Fmm2$	$Fmm2$ $ba2$	$Fmm2$ $ba2$	$F2mm$ $2cb$	$F2mm$ $2cb$	$Fm2m$ $c2a$	$Fm2m$ $c2a$
			$nc2_1$	$nc2_1$	2_1na	2_1an	$b2_1n$	$n2_1b$
			$cn2_1$	$cn2_1$	2_1an	2_1na	$n2_1b$	$b2_1n$
43	C_{2v}^{19}	$Fdd2$	$Fdd2$ $dd2_1$	$Fdd2$ $dd2_1$	$F2dd$ 2_1dd	$F2dd$ 2_1dd	$Fd2d$ $d2_1d$	$Fd2d$ $d2_1d$
44	C_{2v}^{20}	$Imm2$	$Imm2$ $nn2_1$	$Imm2$ $nn2_1$	$I2mm$ 2_1nn	$I2mm$ 2_1nn	$Im2m$ $n2_1n$	$Im2m$ $n2_1n$
45	C_{2v}^{21}	$Iba2$	$Iba2$ $cc2_1$	$Iba2$ $cc2_1$	$I2cb$ 2_1aa	$I2cb$ 2_1aa	$Ic2a$ $b2_1b$	$Ic2a$ $b2_1b$
46	C_{2v}^{22}	$Ima2$	$Ima2$ $nc2_1$	$Ima2$ $nc2_1$	$I2mb$ 2_1na	$I2cm$ 2_1an	$Ic2m$ $b2_1n$	$Im2a$ $n2_1b$
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	$P\frac{2}{b}\frac{2}{a}\frac{2}{-}$	$Pban$	$Pban$	$Pncb$	$Pncb$	$Pcna$	$Pcna$
51	D_{2h}^5	$P\frac{2}{m}\frac{2}{m}\frac{2}{a}$	$Pmma$	$Pmma$	$Pbmm$	$Pbmm$	$Pmcm$	$Pmam$
52	D_{2h}^6	$P\frac{2}{n}\frac{2}{n}\frac{2}{a}$	$Pnna$	$Pnnb$	$Pbnn$	$Pcnn$	$Pncn$	$Pnan$
53	D_{2h}^7	$P\frac{2}{m}\frac{2}{n}\frac{2}{a}$	$Pmna$	$Pnmb$	$Pbmn$	$Pcnm$	$Pncm$	$Pman$
54	D_{2h}^8	$P\frac{2}{c}\frac{2}{c}\frac{2}{a}$	$Pcca$	$Pccb$	$Pbaa$	$Pcaa$	$Pbcb$	$Pbab$
55	D_{2h}^9	$P\frac{2}{b}\frac{2}{a}\frac{2}{m}$	$Pbam$	$Pbam$	$Pmcb$	$Pmcb$	$Pcma$	$Pcma$
56	D_{2h}^{10}	$P\frac{2}{c}\frac{2}{c}\frac{2}{n}$	$Pccn$	$Pccn$	$Pnaa$	$Pnaa$	$Pbnb$	$Pbnb$
57	D_{2h}^{11}	$P\frac{2}{b}\frac{2}{c}\frac{2}{m}$	$Pbcm$	$Pcam$	$Pmca$	$Pmab$	$Pbma$	$Pcmb$
58	D_{2h}^{12}	$P\frac{2}{n}\frac{2}{n}\frac{2}{m}$	$Pnnm$	$Pnnm$	$Pmnn$	$Pmnn$	$Pnmm$	$Pnmm$
59	D_{2h}^{13}	$P\frac{2}{m}\frac{2}{m}\frac{2}{n}$	$Pmmn$	$Pmmn$	$Pnmm$	$Pnmm$	$Pmmn$	$Pmmn$
60	D_{2h}^{14}	$P\frac{2}{b}\frac{2}{c}\frac{2}{n}$	$Pbcn$	$Pcan$	$Pnca$	$Pnab$	$Pbna$	$Pcnb$
61	D_{2h}^{15}	$P\frac{2}{b}\frac{2}{c}\frac{2}{a}$	$Pbca$	$Pcab$	$Pbca$	$Pcab$	$Pbca$	$Pcab$

4. SYNOPTIC TABLES OF SPACE-GROUP SYMBOLS

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)	bac	cab	cba	bca	acb
62	D_{2h}^{16}	$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	<i>Pnma</i>	<i>Pmn</i> <i>bnn</i>	<i>Pbnm</i> <i>ban</i>	<i>Pcmn</i> <i>nae</i>	<i>Pmcn</i> <i>nnn</i>	<i>Pnam</i> <i>nnn</i>
63	D_{2h}^{17}	$C\frac{2}{m}\frac{2}{c}\frac{2}{m}$	<i>Cmcm</i> <i>nan</i>	<i>Cmmm</i> <i>bne</i>	<i>Amma</i> <i>nae</i>	<i>Amam</i> <i>ecn</i>	<i>Bbmm</i> <i>ncb</i>	<i>Bmm</i> <i>cnn</i>
64*†	D_{2h}^{18}	$C\frac{2}{m}\frac{2}{c}\frac{2}{e}$	<i>Cmce</i> <i>bne</i>	<i>Ccme</i> <i>nae</i>	<i>Aema</i> <i>ecn</i>	<i>Aeam</i> <i>enb</i>	<i>Bbem</i> <i>nea</i>	<i>Bmbe</i> <i>cen</i>
65	D_{2h}^{19}	$C\frac{2}{m}\frac{2}{m}\frac{2}{m}$	<i>Cmmm</i> <i>ban</i>	<i>Cmmm</i> <i>ban</i>	<i>Ammm</i> <i>ncb</i>	<i>Anmm</i> <i>ncb</i>	<i>Bmmm</i> <i>cna</i>	<i>Bmmm</i> <i>cna</i>
66	D_{2h}^{20}	$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$	<i>Cccm</i> <i>nnn</i>	<i>Cccm</i> <i>nnn</i>	<i>Amaa</i> <i>nnn</i>	<i>Amaa</i> <i>nnn</i>	<i>Bbmb</i> <i>nnn</i>	<i>Bbmb</i> <i>nnn</i>
67*†	D_{2h}^{21}	$C\frac{2}{m}\frac{2}{m}\frac{2}{e}$	<i>Cmme</i> <i>bae</i>	<i>Cmme</i> <i>bae</i>	<i>Aemm</i> <i>ecb</i>	<i>Aemm</i> <i>ecb</i>	<i>Bmem</i> <i>cea</i>	<i>Bmem</i> <i>cea</i>
68*	D_{2h}^{22}	$C\frac{2}{c}\frac{2}{c}\frac{2}{e}$	<i>Ccce</i> <i>nne</i>	<i>Ccce</i> <i>nne</i>	<i>Aeaa</i> <i>enn</i>	<i>Aeaa</i> <i>enn</i>	<i>Bbeb</i> <i>nen</i>	<i>Bbeb</i> <i>nen</i>
69	D_{2h}^{23}	$F\frac{2}{m}\frac{2}{m}\frac{2}{m}$	<i>Fmmm</i> <i>ban</i>	<i>Fmmm</i> <i>ncb</i>	<i>Fmmm</i> <i>cna</i>	<i>Fmmm</i> <i>ban</i>	<i>Fmmm</i> <i>ncb</i>	<i>Fmmm</i> <i>ban</i>
70	D_{2h}^{24}	$F\frac{2}{d}\frac{2}{d}\frac{2}{d}$	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>
71	D_{2h}^{25}	$I\frac{2}{m}\frac{2}{m}\frac{2}{m}$	<i>I mmm</i> <i>nnn</i>	<i>I mmm</i> <i>nnn</i>	<i>I mmm</i> <i>nnn</i>	<i>I mmm</i> <i>nnn</i>	<i>I mmm</i> <i>nnn</i>	<i>I mmm</i> <i>nnn</i>
72	D_{2h}^{26}	$I\frac{2}{b}\frac{2}{a}\frac{2}{m}$	<i>I bam</i> <i>ccn</i>	<i>I bam</i> <i>ccn</i>	<i>I mcb</i> <i>naa</i>	<i>I mcb</i> <i>naa</i>	<i>I cma</i> <i>bnb</i>	<i>I cma</i> <i>bnb</i>
73	D_{2h}^{27}	$I\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	<i>I bca</i> <i>cab</i>	<i>I cab</i> <i>bca</i>	<i>I bca</i> <i>cab</i>	<i>I cab</i> <i>bca</i>	<i>I bca</i> <i>cab</i>	<i>I cab</i> <i>bca</i>
74†	D_{2h}^{28}	$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}$	<i>I mma</i> <i>nna</i>	<i>I mmb</i> <i>cnn</i>	<i>I bmm</i> <i>bnn</i>	<i>I cmm</i> <i>nan</i>	<i>I mcm</i> <i>nan</i>	<i>I mam</i> <i>ncn</i>

* 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	Schoenflies symbol	Hermann–Mauguin symbols for standard cell <i>P</i> or <i>I</i>		Multiple cell <i>C</i> or <i>F</i>		No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell <i>P</i> or <i>I</i>		Multiple cell <i>C</i> or <i>F</i>	
		Short	Extended	Short	Extended			Short	Extended	Short	Extended
75	C_4^1	<i>P4</i>		<i>C4</i>		83	C_{4h}^1	<i>P4/m</i>		<i>C4/m</i>	<i>C4₂/m</i>
76	C_4^2	<i>P4₁</i>		<i>C4₁</i>		84	C_{4h}^2	<i>P4₂/m</i>		<i>C4₂/m</i>	<i>C4₂/m</i>
77	C_4^3	<i>P4₂</i>		<i>C4₂</i>		85	C_{4h}^3	<i>P4/n</i>		<i>C4/a</i>	<i>C4/a</i>
78	C_4^4	<i>P4₃</i>		<i>C4₃</i>		86	C_{4h}^4	<i>P4₂/n</i>		<i>C4₂/a</i>	<i>C4₂/a</i>
79	C_4^5	<i>I 4</i>	<i>4₂</i>	<i>F4</i>	<i>F4</i>	87	C_{4h}^5	<i>I 4/m</i>	<i>4₂/n</i>	<i>F4/m</i>	<i>F4/m</i>
80	C_4^6	<i>I 4₁</i>	<i>4₃</i>	<i>F4₁</i>	<i>F4₁</i>	88	C_{4h}^6	<i>I 4₁/a</i>	<i>4₃/b</i>	<i>F4₁/d</i>	<i>F4₁/d</i>
81	S_4^1	<i>P₄</i>		<i>C₄</i>							
82	S_4^2	<i>I₄</i>		<i>F₄</i>							

4.3. SYMBOLS FOR SPACE GROUPS

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

TETRAGONAL SYSTEM (*cont.*)

TETRAGONAL SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell <i>P</i> or <i>I</i>		Multiple cell <i>C</i> or <i>F</i>		No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell <i>P</i> or <i>I</i>		Multiple cell <i>C</i> or <i>F</i>	
		Short	Extended	Short	Extended			Short	Extended	Short	Extended
89	D_4^1	$P422$	$P422$ 2_1	$C422$	$C422$ 2_1	119	D_{2d}^9	$I\bar{4}m2$	$I\bar{4}m2$ $n2_1$	$F\bar{4}2m$	$F\bar{4}2m$ 2_{1g2}
90	D_4^2	$P42_12$	$P42_12$ 2_1	$C422_1$	$C422_1$ 2_1	120	D_{2d}^{10}	$I\bar{4}c2$	$I\bar{4}c2$ $b2_1$	$F\bar{4}2c$	$F\bar{4}2c$ 2_{1n}
91	D_4^3	$P4_122$	$P4_122$ 2_1	$C4_122$	$C4_122$ 2_1	121	D_{2d}^{11}	$I\bar{4}2m$	$I\bar{4}2m$ 2_1e	$F\bar{4}m2$	$F\bar{4}m2$ $e2_1$
92	D_4^4	$P4_12_12$	$P4_12_12$ 2_1	$C4_122_1$	$C4_122_1$ 2_1	122	D_{2d}^{12}	$I\bar{4}2d$	$I\bar{4}2d$ 2_1d	$F\bar{4}d2$	$F\bar{4}d2$ $d2_1$
93	D_4^5	$P4_222$	$P4_222$ 2_1	$C4_222$	$C4_222$ 2_1	123	D_{4h}^1	$P4/mmm$	$P4/m 2/m$ $2/m$ $2_1/g$	$C4/mmm$	$C4/mmm$ nb
94	D_4^6	$P4_22_12$	$P4_22_12$ 2_1	$C4_222_1$	$C4_222_1$ 2_1	124	D_{4h}^2	$P4/mcc$	$P4/m 2/c$ $2/c$ $2_1/n$	$C4/mcc$	$C4/mcc$ nn
95	D_4^7	$P4_322$	$P4_322$ 2_1	$C4_322$	$C4_322$ 2_1	125	D_{4h}^3	$P4/nbm$	$P4/n 2/b$ $2/m$ $2_1/g$	$C4/amg_1$	$C4/amg_1$ bb
96	D_4^8	$P4_32_12$	$P4_32_12$ 2_1	$C4_322_1$	$C4_322_1$ 2_1	126	D_{4h}^4	$P4/nnc$	$P4/n 2/n$ $2/c$ $2_1/n$	$C4/acg_2$	$C4/acg_2$ bn
97	D_4^9	$I\bar{4}22$	$I\bar{4}22$ $4_22_12_1$	$F422$	$F422$ $4_22_12_1$	127	D_{4h}^5	$P4/mbm$	$P4/m 2/b$ $2/m$ $2_1/g$	$C4/mmg_1$	$C4/mmg_1$ nb
98	D_4^{10}	$I4_122$	$I4_122$ $4_32_12_1$	$F4_122$	$F4_122$ $4_32_12_1$	128	D_{4h}^6	$P4/mnc$	$P4/m 2_1/n$ $2/c$ $2_1/n$	$C4/mcg_2$	$C4/mcg_2$ nn
99	C_{4v}^1	$P4mm$	$P4mm$ g	$C4mm$	$C4mm$ b	129	D_{4h}^7	$P4/nmm$	$P4/n 2_1/m$ $2/m$ $2_1/g$	$C4/amm$	$C4amm$ bb
100	C_{4v}^2	$P4bm$	$P4bm$ g	$C4mg_1$	$C4mg_1$ b	130	D_{4h}^8	$P4/ncc$	$P4/n 2_1/c$ $2/c$ $2_1/n$	$C4/acc$	$C4/acc$ bn
101	C_{4v}^3	$P4_2cm$	$P4_2cm$ g	$C4_2mc$	$C4_2mc$ b	131	D_{4h}^9	$P4_2/mmc$	$P4_2/m2/m$ $2/c$ $2_1/n$	$C4_2/mcm$	$C4_2/mcm$ nn
102	C_{4v}^4	$P4_2nm$	$P4_2nm$ g	$C4_2mg_2$	$C4_2mg_2$ b	132	D_{4h}^{10}	$P4_2/mcm$	$P4_2/m2/c$ $2/m$ $2_1/g$	$C4_2/mmc$	$C4_2/mmc$ nb
103	C_{4v}^5	$P4cc$	$P4cc$ n	$C4cc$	$C4cc$ n	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
104	C_{4v}^6	$P4nc$	$P4nc$ n	$C4cg_2$	$C4cg_2$ n	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
105	C_{4v}^7	$P4_2mc$	$P4_2mc$ n	$C4_2cm$	$C4_2cm$ n	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
106	C_{4v}^8	$P4_2bc$	$P4_2bc$ n	$C4_2cg_1$	$C4_2cg_1$ n	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
107	C_{4v}^9	$I\bar{4}mm$	$I\bar{4}mm$ 4_2ne	$F4mm$	$F4mm$ 4_2eg_2	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
108	C_{4v}^{10}	$I\bar{4}cm$	$I\bar{4}cm$ 4_2bm	$F4mc$	$F4ec$ 4_2mg_1	138	D_{4h}^{16}	$P4_2/ncm$	$P4_2/n 2_1/c$ $2/m$ $2_1/g$	$C4_2/acm$	$C4_2/acm$ bb
109	C_{4v}^{11}	$I4_1md$	$I4_1md$ 4_1nd	$F4_1dm$	$F4_1dm$ 4_3dg_2	139	D_{4h}^{17}	$I4/mmm$	$I4/m 2/m$ $2/m$ $4_2/n 2_1/n$ $2_1/e$	$F4/mmm$	$F4/mmm$ $4_2/aeg_2$
110	C_{4v}^{12}	$I4_1cd$	$I4_1cd$ 4_3bd	$F4_1dc$	$F4_1dc$ 4_3dg_1	140	D_{4h}^{18}	$I4/mcm$	$I4/m 2/c$ $2/e$ $4_2/n 2_1/b$ $2_1/m$	$F4/mmc$	$F4/mec$
111	D_{2d}^1	$P\bar{4}2m$	$P\bar{4}2m$ g	$C\bar{4}m2$	$C\bar{4}m2$ b	141	D_{4h}^{19}	$I4_1/amd$	$I4_1/a 2/m$ $2/d$ $4_3/b 2_1/n$ $2_1/d$	$F4_1/ddm$	$F4_1/ddm$ $4_3/ddg_2$
112	D_{2d}^2	$P\bar{4}2c$	$P\bar{4}2c$ n	$C\bar{4}c2$	$C\bar{4}c2$ n	142	D_{4h}^{20}	$I4_1/acd$	$I4_1/a 2/c$ $2/d$ $4_3/b 2_1/b$ $2_1/d$	$F4_1/ddc$	$F4_1/ddc$ $4_3/ddg_1$
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	$C\bar{4}c_21$	$C\bar{4}c_21$ 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						

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).

4. SYNOPTIC TABLES OF SPACE-GROUP SYMBOLS

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	$R\bar{3}c$	$R\bar{3}2/c$	$R\bar{3}$ $2/c$ $3_{1,2}2_1/n$	

Example: B $2/b$ 11 (15, unique axis a)

$2_1/n$

The t subgroups of index [2] (type I) are $B211(C2)$; $Bb11(Cc)$; $B\bar{1}(P1)$.

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 $P211(P2)$; $P2_111(P2_1)$; $Pb11(Pc)$; $Pn11(Pc)$; $P\bar{1}$; $B1(P1)$.

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	$P622$			$H622$
178	D_6^2	$P6_122$			$H6_122$
179	D_6^3	$P6_522$			$H6_522$
180	D_6^4	$P6_222$			$H6_222$
181	D_6^5	$P6_422$			$H6_422$
182	D_6^6	$P6_322$			$H6_322$
183	C_{6v}^1	$P6mm$			$H6mm$
184	C_{6v}^2	$P6cc$			$H6cc$
185	C_{6v}^3	$P6_3cm$			$H6_3mc$
186	C_{6v}^4	$P6_3mc$			$H6_3cm$
187	D_{3h}^1	$P\bar{6}m2$			$H\bar{6}2m$
188	D_{3h}^2	$P\bar{6}c2$			$H\bar{6}2c$
189	D_{3h}^3	$P\bar{6}2m$			$H\bar{6}m2$
190	D_{3h}^4	$P\bar{6}2c$			$H\bar{6}c2$
191	D_{6h}^1	$P6/mmm$	$P6/m2/m2/m$	$P6/m2/m2/m$ $2_1/b$ $2_1/a$	$H6/mmm$
192	D_{6h}^2	$P6/mcc$	$P6/m2/c2/c$	$P6/m2/c2/c$ $2_1/n$ $2_1/n$	$H6/mcc$
193	D_{6h}^3	$P6_3/mcm$	$P6_3/m2/c2/m$	$P6_3/m2/c2/m$ $2_1/b$ $2_1/a$	$H6_3/mmc$
194	D_{6h}^4	$P6_3/mmc$	$P6_3/m2/m2/c$	$P6_3/m2/m2/c$ $2_1/b$ $2_1/n$	$H6_3/mcm$

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 \mathbf{a} , \mathbf{b} , \mathbf{c} . In *IT* (1952), left-handed systems like $\bar{\mathbf{c}}\mathbf{b}\mathbf{a}$ were changed to right-handed systems by reversing the orientation of the c axis, as in $\mathbf{c}\mathbf{b}\mathbf{a}$. Note that reversal