

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

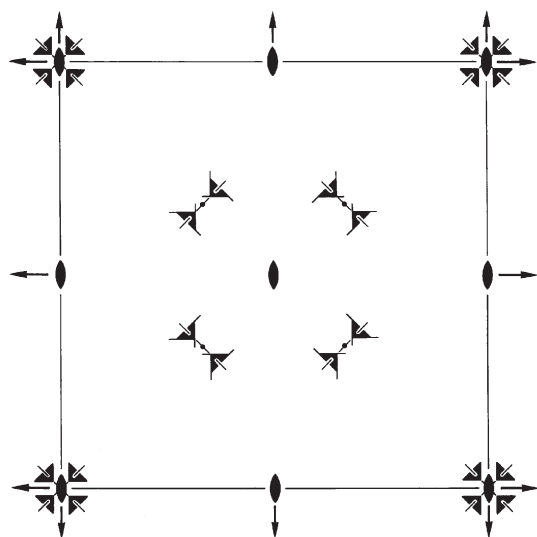


Figure 1.5.4.1
Symmetry-element diagram for space group $P23$ (195).

The analysis illustrates that the combination of the twofold rotation $2x, x, 0$ with I -centring translations gives rise to symmetry elements of rotation and of screw rotation type (cf. Table 1.5.4.2).

Example 5

Let $W = x, y, \bar{z}$ be a reflection $m\ x, y, 0$ with the c axis normal to the reflection plane. An F -centred lattice contains a centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ and the composition of W with this translation is an n glide, since the intrinsic translation part of

$W' = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ is $w'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and consequently the loca-

tion part is $w'_l = \mathbf{o}$. The symmetry operation W' is thus an n glide with the plane $x, y, 0$ as geometric element. However, since the intrinsic translation part w'_g is a lattice vector, W and W' are coplanar equivalents and belong to the element set of the same symmetry element, which is a reflection plane.

The composition of $W = x, y, \bar{z}$ with $t(0, \frac{1}{2}, \frac{1}{2})$ is a b glide, because $W' = x, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ has intrinsic translation part

$w'_g = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$. The location part is $w'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$ and since $(\mathbf{I} - \mathbf{W})\mathbf{p} = w'_l$ for $\mathbf{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, the geometric element of this

glide reflection is the plane $x, y, \frac{1}{4}$. Likewise, the composition $W' = x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ of W with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an a glide with the same plane $x, y, \frac{1}{4}$ as geometric element. The two symmetry operations $b\ x, y, \frac{1}{4}$ and $a\ x, y, \frac{1}{4}$, differing only by the lattice vector $(-\frac{1}{2}, \frac{1}{2}, 0)$ in their translation parts, are coplanar equivalents and belong to the element set of an e -glide plane (cf. Section 1.2.3 for an introduction to e -glide notation).

1.5.4.2. Synoptic table of the plane groups

The possible plane-group symbols are listed in Table 1.5.4.3. Two cases of multiple cells are included in addition to the standard cells, namely the c centring in the square system and the h centring in the hexagonal system. The c centring is defined by

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b}; \quad \mathbf{b}' = \pm \mathbf{a} + \mathbf{b}$$

with centring points at $0, 0$ and $\frac{1}{2}, \frac{1}{2}$. The triple h cell is defined by

$$\mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{a} + 2\mathbf{b}$$

with centring points at $0, 0; \frac{2}{3}, \frac{1}{3}$ and $\frac{1}{3}, \frac{2}{3}$. The glide lines g directly listed under the mirror lines m in the extended and multiple cell symbols indicate that the two symmetry elements are parallel and alternate in the perpendicular direction.

1.5.4.3. Synoptic table of the space groups

Table 1.5.4.4 gives a comprehensive listing of the possible space-group symbols for various settings and choices of the unit cell. The data are ordered according to the crystal systems. The extended Hermann–Mauguin symbols provide information on the additional symmetry operations generated by the compositions of the symmetry operations with lattice translations. An extended Hermann–Mauguin symbol is a complex multi-line symbol: (i) the first line contains those symmetry operations for which the coordinate triplets are explicitly printed under ‘Positions’ in the space-group tables in this volume; (ii) the entries of the lines below indicate the additional symmetry operations generated by the compositions of the symmetry operations of the first line with lattice translations. For example, for A -, B -, C - and I -centred space groups, the entries of the second line of the two-line extended symbol denote the symmetry operations generated by combinations with the corresponding centring translations.³

In the triclinic system the corresponding symbols do not depend on any space direction. Therefore, only the two standard symbols $P1$ (1) and $\bar{P}1$ (2) are listed. One should, however, bear in mind that in some circumstances it might be more appropriate to use a centred cell for comparison purposes, e.g. following a phase transition resulting from a temperature, pressure or composition change.

The monoclinic and orthorhombic systems present the largest number of alternatives owing to various settings and cell choices. In the monoclinic system, three choices of unique axis can occur, namely b , c and a . In each case, two permutations of the other axes are possible, thus yielding six possible settings given in terms of three pairs, namely \underline{abc} and \underline{cba} , \underline{abc} and \underline{bac} , \underline{abc} and \underline{acb} . The unique axes are underlined and the negative sign, placed over the letter, maintains the correct handedness of the reference system. The three possible cell choices indicated in Fig. 1.5.3.1 increase the number of possible symbols by a factor of three, thus yielding 18 different cases for each monoclinic space group, except for five cases, namely $P2$ (3), $P2_1$ (4), Pm (6), $P2/m$ (10) and $P2_1/m$ (11) with only six variants.

In monoclinic P lattices, the symmetry operations along the symmetry direction are always unique. Here again, as in the plane groups, the cell centring gives rise to additional entries in the extended Hermann–Mauguin symbols. Consider, for example, the data for monoclinic $P12/m1$ (10), $C12/m1$ (12) and $C12/c1$ (15) in Table 1.5.4.4. For $P12/m1$ and its various settings there is only one line, which corresponds to the full Hermann–Mauguin symbols; these contain only rotations 2 and reflections m . The first line for $C12/m1$ is followed by a second line, the first entry of which is the symbol $2_1/a$, because 2_1 screw rotations and a glide reflections also belong to this space group. Similarly, in $C12/c1$

³ After the introduction of the e -glide convention and the symmetry-element interpretation of the characters of the Hermann–Mauguin symbols (de Wolff *et al.*, 1992), the tabulated data for the extended symbols were partially modified by introducing the e -glide notation in the symbols of only some of the groups [cf. Table 4.3.2.1 of the fifth edition of *IT A* (2002)]. In contrast to the fifth edition, in Table 1.5.4.4 extended symbols similar to those that can be found in the first four editions of *IT A* have been reinstated.

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.5.4.3

List of plane-group symbols

System and lattice symbol	Point group	No. of plane group	Hermann–Mauguin symbol			Full symbol for other setting	Multiple cell
			Short	Full	Extended		
Oblique <i>p</i>	1	1		<i>p1</i>			
	2	2		<i>p2</i>			
Rectangular <i>p, c</i>	<i>m</i>	{ 3 4 5	<i>pm</i>	<i>p1m1</i>	<i>c1m1</i> <i>g</i>	<i>p11m</i>	
			<i>pg</i>	<i>p1g1</i>		<i>p11g</i>	
<i>cm</i>			<i>c1m1</i>	<i>c11m</i>			
	<i>2mm</i>	{ 6 7 8 9		<i>p2mm</i>	<i>c2mm</i> <i>g g</i>	<i>p2mm</i>	
			<i>p2mg</i>	<i>p2gm</i>			
			<i>p2gg</i>	<i>p2gg</i>			
			<i>c2mm</i>	<i>c2mm</i>			
Square <i>p</i>	4	10		<i>p4</i>	<i>p4mm</i> <i>g</i> <i>p4gm</i> <i>g</i>		<i>c4</i>
	<i>4mm</i>	{ 11 12		<i>p4mm</i>			<i>c4mm</i>
				<i>p4gm</i>			<i>g</i> <i>c4mg</i> <i>g</i>
Hexagonal <i>p</i>	3	13		<i>p3</i>	<i>p3m1</i> <i>g</i> <i>p31m</i> <i>g</i> <i>p6</i> <i>p6mm</i> <i>g g</i>		<i>h3</i>
	<i>3m</i>	{ 14 15		<i>p3m1</i>			<i>h31m</i>
				<i>p31m</i>			<i>g</i> <i>h3m1</i>
				<i>p6</i>			<i>g</i> <i>h6</i>
	<i>6</i>	16		<i>p6mm</i>			<i>h6mm</i>
<i>6mm</i>	17		<i>g g</i>	<i>g g</i>			

rotations 2 and screw rotations 2_1 and c and n glide reflections alternate, and thus under the full symbol $C12/c1$ one finds the entry $2_1/n$.

In Table 1.5.4.4 the Hermann–Mauguin symbols of the orthorhombic space groups are listed in six different settings: the *standard setting abc*, and the settings *ba \bar{c}* , *cab*, *$\bar{c}ba$* , *bca* and *a $\bar{c}b$* . These six settings result from the possible permutations of the three axes. Let us compare for a few space groups the standard setting *abc* with the *cab* setting. For $Pmm2$ (25) the permutation yields the new setting $P2mm$, reflecting the fact that the twofold axes parallel to the c direction change to the a direction. The mirrors normal to a and b become normal to b and c , respectively.

The case of $Cmm2$ (35) is slightly more complex due to the centring. As a result of the permutation the C centring becomes an A centring. The changes in the twofold axes and mirrors are similar to those of the previous example and result in the $A2mm$ setting of $Cmm2$.

The extended Hermann–Mauguin symbol of the centred space group $Aem2$ (39) reveals the nature of the e -glide plane (also called the ‘double’ glide plane): among the set of glide reflections through the same (100) plane, there exist two glide reflections with glide components $\frac{1}{2}b$ and $\frac{1}{2}c$ (for details of the e -glide notation the reader is referred to Section 1.2.3, see also de Wolff *et al.*, 1992). In the *cab* setting, the A centring changes to a B centring and the double glide plane is now normal to b and the glide reflections have glide components $\frac{1}{2}a$ and $\frac{1}{2}c$. The corresponding symbol is thus $B2em$. Note that in the cases of the five orthorhombic space groups whose Hermann–Mauguin symbols contain the e -glide symbol, namely $Aem2$ (39), $Aea2$ (41), $Cmce$ (64), $Cmme$ (67) and $Ccce$ (68), the characters in the first lines of the extended symbols differ from the short symbols because the characters in the extended symbol represent symmetry operations, whereas those in the short and full symbol represent symmetry elements. In all these cases, the extended symbols

listed in Table 1.5.4.4 are complemented by the short symbols, given in brackets.

The general discussion in Section 1.5.4.1 about the additional symmetry operations that occur as a result of combinations with lattice translations provides some rules for the construction of the extended Hermann–Mauguin symbols in the orthorhombic crystal system. In orthorhombic space groups with primitive lattices, the symmetry operations of any symmetry direction are always unique: either 2 or 2_1 , either m or a or b or c or n . In C -centred lattices, owing to the possible combination of the original symmetry operations with the centring translations, the axes 2 along [100] and [010] alternate with axes 2_1 . However, parallel to c there are either 2 or 2_1 axes because the combination of a rotation or screw rotation with a centring translation results in another operation of the same kind. Similarly, m_{100} alternates with b_{100} , m_{010} with a_{010} , c_{100} with n_{100} etc. The m_{001} reflection plane is simultaneously an n_{001} glide plane and an a_{001} glide plane is simultaneously a b_{001} glide plane. This latter plane with its double role is the e_{001} glide plane, as found for example in the full symbol of $C2/m2/m2/e$ (67) and the corresponding short symbol $Cmme$. As another example, consider the space group $C2/m2/c2_1/m$ (63). In Table 1.5.4.4, in the line of various settings for this space group the short Hermann–Mauguin symbols are listed, and the rotations or screw rotations do not appear. The m_{100} , c_{010} and m_{001} reflections and glide reflections occur alternating with b_{100} , n_{010} and n_{001} glide reflections, respectively. The entry under $Cmcm$ is thus bnn .

F and I centring cause alternating symmetry operations for all three coordinate axes a , b and c . For these centring, the permutation of the axes does not affect the symbol F or I of the centring type. However, the number of symmetry operations increases by a factor of four for F centring and by a factor of two for I centring when compared to those of a space group with a

(continued on page 106)

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Table 1.5.4.4

List of space-group symbols 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						Unique axis <i>b</i> Unique axis <i>c</i> Unique axis <i>a</i>	
			\underline{abc}	\bar{cba}	\underline{abc}	$\underline{ba\bar{c}}$	\underline{abc}	$\bar{a\bar{c}b}$		
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	$C2$	$C121$	$A121$	$A112$	$B112$	$B211$	$C211$	Cell choice 1	
			2_1	2_1	2_1	2_1	2_1	2_1	Cell choice 2	
			$A121$	$C121$	$B112$	$A112$	$C211$	$B211$	2_1	Cell choice 3
			$I121$	$I121$	$I112$	$I112$	$I211$	$I211$		
			2_1	2_1	2_1	2_1	2_1	2_1		
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	
8	C_s^3	Cm	$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3	
			$C1m1$	$A1m1$	$A11m$	$B11m$	$Bm11$	$Cm11$	Cell choice 1	
			a	c	b	a	b	c	Cell choice 2	
			$A1m1$	$C1m1$	$B11m$	$A11m$	$Cm11$	$Bm11$		
			c	a	a	b	b	c		
			$I1m1$	$I1m1$	$I11m$	$I11m$	$Im11$	$Im11$	Cell choice 3	
9	C_s^4	Cc	n	n	n	n	n	n	Cell choice 1	
			$C1c1$	$A1a1$	$A11a$	$B11b$	$Bb11$	$Cc11$	$Cc11$	Cell choice 2
			n	n	n	n	n	n	n	Cell choice 3
			$A1n1$	$C1n1$	$B11n$	$A11n$	$Cn11$	$Bn11$		
			a	c	b	a	c	b		
			$I1a1$	$I1c1$	$I11b$	$I11a$	$Ic11$	$Ib11$		
			c	a	a	b	b	c		
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	$C2/m$	$C1\frac{2}{m}1$	$A1\frac{2}{m}1$	$A11\frac{2}{m}$	$B11\frac{2}{m}$	$B\frac{2}{m}11$	$C\frac{2}{m}11$	Cell choice 1	
			$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$		
			$A1\frac{2}{m}1$	$C1\frac{2}{m}1$	$B11\frac{2}{m}$	$A11\frac{2}{m}$	$C\frac{2}{m}11$	$B\frac{2}{m}11$	Cell choice 2	
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$		
			$I1\frac{2}{m}1$	$I1\frac{2}{m}1$	$I11\frac{2}{m}$	$I11\frac{2}{m}$	$I\frac{2}{m}11$	$I\frac{2}{m}11$	Cell choice 3	
			$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$		
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	

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.5.4.4 (continued)

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>
			\underline{abc}	\underline{cba}	\underline{abc}	$\underline{ba\bar{c}}$	\underline{abc}	$\underline{a\bar{c}b}$	
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	$C2/c$	$C1\frac{2}{c}1$	$A1\frac{2}{a}1$	$A11\frac{2}{a}$	$B11\frac{2}{b}$	$B\frac{2}{b}11$	$C\frac{2}{c}11$	Cell choice 1
			$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	
			$A1\frac{2}{n}1$	$C1\frac{2}{n}1$	$B11\frac{2}{n}$	$A11\frac{2}{n}$	$C\frac{2}{n}11$	$B\frac{2}{n}11$	Cell choice 2
			$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	
			$I1\frac{2}{a}1$	$I1\frac{2}{c}1$	$I11\frac{2}{b}$	$I11\frac{2}{a}$	$I\frac{2}{c}11$	$I\frac{2}{b}11$	Cell choice 3
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$	
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$	

ORTHORHOMBIC SYSTEM

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol \underline{abc}	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			\underline{abc} (standard)	$\underline{ba\bar{c}}$	\underline{cab}	\underline{cba}	\underline{bca}	$\underline{a\bar{c}b}$
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	$C222_1$	$C222_1$	$C222_1$	$A2_122$	$A2_122$	$B22_12$	$B22_12$
			$2_12_12_1$	$2_12_12_1$	$2_12_12_1$	$2_12_12_1$	$2_12_12_1$	$2_12_12_1$
21	D_2^6	$C222$	$C222$	$C222$	$A222$	$A222$	$B222$	$B222$
			2_12_12	2_12_12	22_12_1	22_12_1	2_122_1	2_122_1
22	D_2^7	$F222$	$F222$	$F222$	$F222$	$F222$	$F222$	$F222$
			2_12_12	2_12_12	22_12_1	22_12_1	2_122_1	2_122_1
			22_12_1	2_122_1	2_122_1	2_12_12	2_12_12	22_12_1
			2_122_1	22_12_1	2_12_12	2_122_1	22_12_1	2_12_12
23	D_2^8	$I222$	$I222$	$I222$	$I222$	$I222$	$I222$	$I222$
			$2_12_12_1$	$2_12_12_1$	$2_12_12_1$	$2_12_12_1$	$2_12_12_1$	$2_12_12_1$
24	D_2^9	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$
			222	222	222	222	222	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}	$Pnn2$	$Pnn2$	$Pnn2$	$P2nn$	$P2nn$	$Pn2n$	$Pn2n$
35	C_{2v}^{11}	$Cmm2$	$Cmm2$	$Cmm2$	$A2mm$	$A2mm$	$Bm2m$	$Bm2m$
			$ba2$	$ba2$	$2cb$	$2cb$	$c2a$	$c2a$

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

Table 1.5.4.4 (continued)

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}	cab	$\bar{c}ba$	bca	a$\bar{c}b$
36	C_{2v}^{12}	<i>Cmc</i> 2 ₁	<i>Cmc</i> 2 ₁ <i>bn</i> 2 ₁	<i>Ccm</i> 2 ₁ <i>na</i> 2 ₁	<i>A</i> 2 ₁ <i>ma</i> <i>2</i> ₁ <i>cn</i>	<i>A</i> 2 ₁ <i>am</i> <i>2</i> ₁ <i>nb</i>	<i>Bb</i> 2 ₁ <i>m</i> <i>n</i> 2 ₁ <i>a</i>	<i>Bm</i> 2 ₁ <i>b</i> <i>c</i> 2 ₁ <i>n</i>
37	C_{2v}^{13}	<i>Ccc</i> 2	<i>Ccc</i> 2 <i>nn</i> 2	<i>Ccc</i> 2 <i>nn</i> 2	<i>A</i> 2 ₁ <i>aa</i> <i>2nn</i>	<i>A</i> 2 ₁ <i>aa</i> <i>2nn</i>	<i>Bb</i> 2 ₁ <i>b</i> <i>n</i> 2 ₁ <i>n</i>	<i>Bb</i> 2 ₁ <i>b</i> <i>n</i> 2 ₁ <i>n</i>
38	C_{2v}^{14}	<i>Amm</i> 2	<i>Amm</i> 2 <i>nc</i> 2 ₁	<i>Bmm</i> 2 <i>cn</i> 2 ₁	<i>B</i> 2 ₁ <i>mm</i> <i>2</i> ₁ <i>na</i>	<i>C</i> 2 ₁ <i>mm</i> <i>2</i> ₁ <i>an</i>	<i>Cm</i> 2 ₁ <i>m</i> <i>b</i> 2 ₁ <i>n</i>	<i>Am</i> 2 ₁ <i>m</i> <i>n</i> 2 ₁ <i>b</i>
39†	C_{2v}^{15}	<i>Aem</i> 2	<i>Abm</i> 2 (<i>Aem</i> 2) <i>cc</i> 2 ₁	<i>Bma</i> 2 (<i>Bme</i> 2) <i>cc</i> 2 ₁	<i>B</i> 2 ₁ <i>cm</i> (<i>B2em</i>) <i>2</i> ₁ <i>aa</i>	<i>C</i> 2 ₁ <i>mb</i> (<i>C2me</i>) <i>2</i> ₁ <i>aa</i>	<i>Cm</i> 2 ₁ <i>a</i> (<i>Cm2e</i>) <i>b</i> 2 ₁ <i>b</i>	<i>Ac</i> 2 ₁ <i>m</i> (<i>Ae2m</i>) <i>b</i> 2 ₁ <i>b</i>
40	C_{2v}^{16}	<i>Ama</i> 2	<i>Ama</i> 2 <i>nn</i> 2 ₁	<i>Bbm</i> 2 <i>nn</i> 2 ₁	<i>B</i> 2 ₁ <i>mb</i> <i>2</i> ₁ <i>nn</i>	<i>C</i> 2 ₁ <i>cm</i> <i>2</i> ₁ <i>nn</i>	<i>Cc</i> 2 ₁ <i>m</i> <i>n</i> 2 ₁ <i>n</i>	<i>Am</i> 2 ₁ <i>a</i> <i>n</i> 2 ₁ <i>n</i>
41†	C_{2v}^{17}	<i>Aea</i> 2	<i>Aba</i> 2 (<i>Aea</i> 2) <i>cn</i> 2 ₁	<i>Bba</i> 2 (<i>Bbe</i> 2) <i>nc</i> 2 ₁	<i>B</i> 2 ₁ <i>cb</i> (<i>B2eb</i>) <i>2</i> ₁ <i>an</i>	<i>C</i> 2 ₁ <i>cb</i> (<i>C2ce</i>) <i>2</i> ₁ <i>na</i>	<i>Cc</i> 2 ₁ <i>a</i> (<i>Cc2e</i>) <i>n</i> 2 ₁ <i>b</i>	<i>Ac</i> 2 ₁ <i>a</i> (<i>Ae2a</i>) <i>b</i> 2 ₁ <i>n</i>
42	C_{2v}^{18}	<i>Fmm</i> 2	<i>Fmm</i> 2 <i>ba</i> 2 <i>nc</i> 2 ₁ <i>cn</i> 2 ₁	<i>Fmm</i> 2 <i>ba</i> 2 <i>cn</i> 2 ₁ <i>nc</i> 2 ₁	<i>F</i> 2 ₁ <i>mm</i> <i>2cb</i> <i>2</i> ₁ <i>na</i> <i>2</i> ₁ <i>an</i>	<i>F</i> 2 ₁ <i>mm</i> <i>2cb</i> <i>2</i> ₁ <i>an</i> <i>2</i> ₁ <i>na</i>	<i>Fm</i> 2 ₁ <i>m</i> <i>c</i> 2 ₁ <i>a</i> <i>b</i> 2 ₁ <i>n</i> <i>n</i> 2 ₁ <i>b</i>	<i>Fm</i> 2 ₁ <i>m</i> <i>c</i> 2 ₁ <i>a</i> <i>n</i> 2 ₁ <i>b</i> <i>b</i> 2 ₁ <i>n</i>
43	C_{2v}^{19}	<i>Fdd</i> 2	<i>Fdd</i> 2 <i>dd</i> 2 ₁	<i>Fdd</i> 2 <i>dd</i> 2 ₁	<i>F</i> 2 ₁ <i>dd</i> <i>2</i> ₁ <i>dd</i>	<i>F</i> 2 ₁ <i>dd</i> <i>2</i> ₁ <i>dd</i>	<i>Fd</i> 2 ₁ <i>d</i> <i>d</i> 2 ₁ <i>d</i>	<i>Fd</i> 2 ₁ <i>d</i> <i>d</i> 2 ₁ <i>d</i>
44	C_{2v}^{20}	<i>Imm</i> 2	<i>Imm</i> 2 <i>nn</i> 2 ₁	<i>Imm</i> 2 <i>nn</i> 2 ₁	<i>I</i> 2 ₁ <i>mm</i> <i>2</i> ₁ <i>nn</i>	<i>I</i> 2 ₁ <i>mm</i> <i>2</i> ₁ <i>nn</i>	<i>Im</i> 2 ₁ <i>m</i> <i>n</i> 2 ₁ <i>n</i>	<i>Im</i> 2 ₁ <i>m</i> <i>n</i> 2 ₁ <i>n</i>
45	C_{2v}^{21}	<i>Iba</i> 2	<i>Iba</i> 2 <i>cc</i> 2 ₁	<i>Iba</i> 2 <i>cc</i> 2 ₁	<i>I</i> 2 ₁ <i>cb</i> <i>2</i> ₁ <i>aa</i>	<i>I</i> 2 ₁ <i>cb</i> <i>2</i> ₁ <i>aa</i>	<i>Ic</i> 2 ₁ <i>a</i> <i>b</i> 2 ₁ <i>b</i>	<i>Ic</i> 2 ₁ <i>a</i> <i>b</i> 2 ₁ <i>b</i>
46	C_{2v}^{22}	<i>Ima</i> 2	<i>Ima</i> 2 <i>nc</i> 2 ₁	<i>Ibm</i> 2 <i>cn</i> 2 ₁	<i>I</i> 2 ₁ <i>mb</i> <i>2</i> ₁ <i>na</i>	<i>I</i> 2 ₁ <i>cm</i> <i>2</i> ₁ <i>an</i>	<i>Ic</i> 2 ₁ <i>m</i> <i>b</i> 2 ₁ <i>n</i>	<i>Im</i> 2 ₁ <i>a</i> <i>n</i> 2 ₁ <i>b</i>
47	D_{2h}^1	$P \frac{2}{m} \frac{2}{m} \frac{2}{m}$	<i>Pmmm</i>	<i>Pmmm</i>	<i>Pmmm</i>	<i>Pmmm</i>	<i>Pmmm</i>	<i>Pmmm</i>
48	D_{2h}^2	$P \frac{2}{n} \frac{2}{n} \frac{2}{n}$	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>	<i>Pnnn</i>
49	D_{2h}^3	$P \frac{2}{c} \frac{2}{c} \frac{2}{m}$	<i>Pccm</i>	<i>Pccm</i>	<i>Pmaa</i>	<i>Pmaa</i>	<i>Pbmb</i>	<i>Pbmb</i>
50	D_{2h}^4	$P \frac{2}{b} \frac{2}{a} \frac{2}{n}$	<i>Pban</i>	<i>Pban</i>	<i>Pncb</i>	<i>Pncb</i>	<i>Pcna</i>	<i>Pcna</i>
51	D_{2h}^5	$P \frac{2}{m} \frac{2}{m} \frac{2}{a}$	<i>Pmma</i>	<i>Pmmb</i>	<i>Pbmm</i>	<i>Pcmm</i>	<i>Pmcm</i>	<i>Pmam</i>
52	D_{2h}^6	$P \frac{2}{n} \frac{2}{n} \frac{2}{a}$	<i>Pnna</i>	<i>Pnnb</i>	<i>Pbnn</i>	<i>Pcnn</i>	<i>Pncn</i>	<i>Pnan</i>
53	D_{2h}^7	$P \frac{2}{m} \frac{2}{n} \frac{2}{a}$	<i>Pmna</i>	<i>Pnmb</i>	<i>Pbmn</i>	<i>Pcnm</i>	<i>Pncm</i>	<i>Pman</i>
54	D_{2h}^8	$P \frac{2}{c} \frac{2}{c} \frac{2}{a}$	<i>Pcca</i>	<i>Pccb</i>	<i>Pbaa</i>	<i>Pcaa</i>	<i>Pbcb</i>	<i>Pbab</i>
55	D_{2h}^9	$P \frac{2}{b} \frac{2}{a} \frac{2}{m}$	<i>Pbam</i>	<i>Pbam</i>	<i>Pmcb</i>	<i>Pmcb</i>	<i>Pcma</i>	<i>Pcma</i>
56	D_{2h}^{10}	$P \frac{2}{c} \frac{2}{c} \frac{2}{n}$	<i>Pccn</i>	<i>Pccn</i>	<i>Pnaa</i>	<i>Pnaa</i>	<i>Pbnb</i>	<i>Pbnb</i>
57	D_{2h}^{11}	$P \frac{2}{b} \frac{2}{c} \frac{2}{m}$	<i>Pbcm</i>	<i>Pcam</i>	<i>Pmca</i>	<i>Pmab</i>	<i>Pbma</i>	<i>Pcmb</i>
58	D_{2h}^{12}	$P \frac{2}{n} \frac{2}{n} \frac{2}{m}$	<i>Pnnm</i>	<i>Pnnm</i>	<i>Pmnn</i>	<i>Pmnn</i>	<i>Pnmn</i>	<i>Pnmn</i>
59	D_{2h}^{13}	$P \frac{2}{m} \frac{2}{m} \frac{2}{n}$	<i>Pmnn</i>	<i>Pmnn</i>	<i>Pnmm</i>	<i>Pnmm</i>	<i>Pnmn</i>	<i>Pnmn</i>
60	D_{2h}^{14}	$P \frac{2}{b} \frac{2}{c} \frac{2}{n}$	<i>Pbcn</i>	<i>Pcan</i>	<i>Pnca</i>	<i>Pnab</i>	<i>Pbna</i>	<i>Pcnb</i>
61	D_{2h}^{15}	$P \frac{2}{b} \frac{2}{c} \frac{2}{a}$	<i>Pbca</i>	<i>Pcab</i>	<i>Pbca</i>	<i>Pcab</i>	<i>Pbca</i>	<i>Pcab</i>
62	D_{2h}^{16}	$P \frac{2}{n} \frac{2}{m} \frac{2}{a}$	<i>Pnma</i>	<i>Pmnb</i>	<i>Pbnm</i>	<i>Pcmm</i>	<i>Pmcn</i>	<i>Pnam</i>
63	D_{2h}^{17}	$C \frac{2}{m} \frac{2}{c} \frac{2}{m}$	<i>Cmcm</i> <i>bn</i> n	<i>Ccmm</i> <i>nan</i>	<i>Amma</i> <i>ncn</i>	<i>Amam</i> <i>nnb</i>	<i>Bbmm</i> <i>nna</i>	<i>Bmmb</i> <i>cnn</i>
64†	D_{2h}^{18}	$C \frac{2}{m} \frac{2}{c} \frac{2}{e}$	<i>Cmca</i> (<i>Cmce</i>) <i>bn</i> b	<i>Ccmb</i> (<i>Ccme</i>) <i>naa</i>	<i>Abma</i> (<i>Aema</i>) <i>ccn</i>	<i>Acam</i> (<i>Aeam</i>) <i>bn</i> b	<i>Bbcm</i> (<i>Bbem</i>) <i>naa</i>	<i>Bmab</i> (<i>Bmeb</i>) <i>cnn</i>

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.5.4.4 (continued)

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}	cab	$\bar{c}ba$	bca	a$\bar{c}b$
65	D_{2h}^{19}	$C \frac{2\ 2\ 2}{m\ m\ m}$	<i>Cmmm</i> <i>ban</i>	<i>Cmmm</i> <i>ban</i>	<i>Ammm</i> <i>ncb</i>	<i>Ammm</i> <i>ncb</i>	<i>Bmmm</i> <i>cna</i>	<i>Bmmm</i> <i>cna</i>
66	D_{2h}^{20}	$C \frac{2\ 2\ 2}{c\ c\ m}$	<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}	$C \frac{2\ 2\ 2}{m\ m\ e}$	<i>Cmma</i> (<i>Cmme</i>) <i>bab</i>	<i>Cmmb</i> (<i>Cmme</i>) <i>baa</i>	<i>Abmm</i> (<i>Aemm</i>) <i>ccb</i>	<i>Acmm</i> (<i>Aemm</i>) <i>bc b</i>	<i>Bmcm</i> (<i>Bmem</i>) <i>caa</i>	<i>Bmam</i> (<i>Bmem</i>) <i>cca</i>
68†	D_{2h}^{22}	$C \frac{2\ 2\ 2}{c\ c\ e}$	<i>Ccca</i> (<i>Ccce</i>) <i>n nb</i>	<i>Cccb</i> (<i>Ccce</i>) <i>n na</i>	<i>Abaa</i> (<i>Aeaa</i>) <i>c nn</i>	<i>Acaa</i> (<i>Aeaa</i>) <i>b nn</i>	<i>Bbcb</i> (<i>Bbeb</i>) <i>nan</i>	<i>Bbab</i> (<i>Bbeb</i>) <i>nc n</i>
69	D_{2h}^{23}	$F \frac{2\ 2\ 2}{m\ m\ m}$	<i>Fmmm</i> <i>ban</i> <i>nc b</i> <i>c na</i>	<i>Fmmm</i> <i>ban</i> <i>c na</i> <i>nc b</i>	<i>Fmmm</i> <i>nc b</i> <i>c na</i> <i>ban</i>	<i>Fmmm</i> <i>nc b</i> <i>ban</i> <i>c na</i>	<i>Fmmm</i> <i>c na</i> <i>ban</i> <i>nc b</i>	<i>Fmmm</i> <i>c na</i> <i>nc b</i> <i>ban</i>
70	D_{2h}^{24}	$F \frac{2\ 2\ 2}{d\ d\ d}$	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>	<i>Fddd</i>
71	D_{2h}^{25}	$I \frac{2\ 2\ 2}{m\ m\ m}$	<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}	$I \frac{2\ 2\ 2}{b\ a\ m}$	<i>I bam</i> <i>cc n</i>	<i>I bam</i> <i>cc n</i>	<i>I mcb</i> <i>na a</i>	<i>I mcb</i> <i>na a</i>	<i>I cma</i> <i>b nb</i>	<i>I cma</i> <i>b nb</i>
73	D_{2h}^{27}	$I \frac{2_1\ 2_1\ 2_1}{b\ c\ a}$	<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}	$I \frac{2_1\ 2_1\ 2_1}{m\ m\ a}$	<i>I mma</i> <i>n nb</i>	<i>I mmb</i> <i>n na</i>	<i>I bmm</i> <i>c nn</i>	<i>I cmm</i> <i>b nn</i>	<i>I mcm</i> <i>na n</i>	<i>I mam</i> <i>nc n</i>

† For the five space groups *Aem2* (39), *Aea2* (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 (1995). For further explanations, see Sections 1.2.3 and 2.1.2, and de Wolff *et al.* (1992).

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>	
		Short	Extended	Short	Extended
75	C_4^1	<i>P4</i>		<i>C4</i>	
76	C_4^2	<i>P4₁</i>		<i>C4₁</i>	
77	C_4^3	<i>P4₂</i>		<i>C4₂</i>	
78	C_4^4	<i>P4₃</i>		<i>C4₃</i>	
79	C_4^5	<i>I4</i>	<i>I4</i> <i>4₂</i>	<i>F4</i>	<i>F4</i> <i>4₂</i>
80	C_4^6	<i>I4₁</i>	<i>I4₁</i> <i>4₃</i>	<i>F4₁</i>	<i>F4₁</i> <i>4₃</i>
81	S_4^1	<i>P$\bar{4}$</i>		<i>C$\bar{4}$</i>	
82	S_4^2	<i>I$\bar{4}$</i>		<i>F$\bar{4}$</i>	
83	C_{4h}^1	<i>P4/m</i>		<i>C4/m</i>	<i>C4₂/m</i> <i>n</i>
84	C_{4h}^2	<i>P4₂/m</i>		<i>C4₂/m</i>	<i>C4₂/m</i> <i>n</i>
85	C_{4h}^3	<i>P4/n</i>		<i>C4/e</i>	<i>C4/a</i> <i>b</i>
86	C_{4h}^4	<i>P4₂/n</i>		<i>C4₂/e</i>	<i>C4₂/a</i> <i>b</i>
87	C_{4h}^5	<i>I4/m</i>	<i>I4/m</i> <i>4₂/n</i>	<i>F4/m</i>	<i>F4/m</i> <i>4₂/a</i>
88	C_{4h}^6	<i>I4₁/a</i>	<i>I4₁/a</i> <i>4₃/b</i>	<i>F4₁/d</i>	<i>F4₁/d</i> <i>4₃/d</i>
89	D_4^1	<i>P422</i>	<i>P422</i> <i>2₁</i>	<i>C422</i>	<i>C422</i> <i>2₁</i>
90	D_4^2	<i>P42₁2</i>	<i>P42₁2</i> <i>2₁</i>	<i>C422₁</i>	<i>C422₁</i> <i>2₁</i>

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

Table 1.5.4.4 (continued)

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
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_2nc	$F4mm$	$F4mm$ 4_2cg_2
108	C_{4v}^{10}	$I4cm$	$I4cc$ 4_2bm	$F4mc$	$F4cc$ 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
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_1c	$F\bar{4}m2$	$F\bar{4}m2$ $c2_1$
122	D_{2d}^{12}	$I\bar{4}2d$	$I\bar{4}2d$ 2_1d	$F\bar{4}d2$	$F\bar{4}d2$ $d2_1$

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.5.4.4 (continued)

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
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	$P4/nbm$	$P4/n\ 2/b\ 2/m\ 2_1/g$	$C4/emg_1$	$C4/amg_1\ bb$
126	D_{4h}^4	$P4/nnc$	$P4/n\ 2/n\ 2/c\ 2_1/n$	$C4/ecg_2$	$C4/acg_2\ bn$
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	$P4/nmm$	$P4/n\ 2_1/m\ 2/m\ 2_1/g$	$C4/emm$	$C4amm\ bb$
130	D_{4h}^8	$P4/ncc$	$P4/n\ 2_1/c\ 2/c\ 2_1/n$	$C4/ecc$	$C4/acc\ bn$
131	D_{4h}^9	$P4_2/mmc$	$P4_2/m\ 2/m\ 2/c\ 2_1/n$	$C4_2/mcm$	$C4_2/mcm\ nn$
132	D_{4h}^{10}	$P4_2/mcm$	$P4_2/m\ 2/c\ 2/m\ 2_1/g$	$C4_2/mmc$	$C4_2/mmc\ nb$
133	D_{4h}^{11}	$P4_2/nbc$	$P4_2/n\ 2/b\ 2/c\ 2_1/n$	$C4_2/ecg_1$	$C4_2/acg_1\ bn$
134	D_{4h}^{12}	$P4_2/nnm$	$P4_2/n\ 2/n\ 2/m\ 2_1/g$	$C4_2/emg_2$	$C4_2/amg_2\ bb$
135	D_{4h}^{13}	$P4_2/mbc$	$P4_2/m\ 2_1/b\ 2/c\ 2_1/n$	$C4_2/mcg_1$	$C4_2/mcg_1\ nn$
136	D_{4h}^{14}	$P4_2/mnm$	$P4_2/m\ 2_1/n\ 2/m\ 2_1/g$	$C4_2/mmg_2$	$C4_2/mmg_2\ nb$
137	D_{4h}^{15}	$P4_2/nmc$	$P4_2/n\ 2_1/m\ 2/c\ 2_1/n$	$C4_2/ecm$	$C4_2/acm\ bn$
138	D_{4h}^{16}	$P4_2/ncm$	$P4_2/n\ 2_1/c\ 2/m\ 2_1/g$	$C4_2/emc$	$C4_2/amc\ bb$
139	D_{4h}^{17}	$I4/mmm$	$I4/m\ 2/m\ 2/m\ 4_2/n\ 2_1/n\ 2_1/c$	$F4/mmm$	$F4/mmm\ 4_2/acg_2$
140	D_{4h}^{18}	$I4/mcm$	$I4/m\ 2/c\ 2/c\ 4_2/n\ 2_1/b\ 2_1/m$	$F4/mmc$	$F4/mcc\ 4_2/amg_1$
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 Sections 1.2.3 and 2.1.2, and de Wolff *et al.* (1992).

TRIGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell <i>P</i> or <i>R</i>			Triple cell <i>H</i>
		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	$\bar{P}3$			$\bar{H}3$
148	C_{3i}^2	$\bar{R}3$		$\bar{R}3\ 3_{1,2}$	
149	D_3^1	$P312$		$P312\ 2_1$	$H321$
150	D_3^2	$P321$		$P321\ 2_1$	$H312$
151	D_3^3	$P3_112$		$P3_112\ 2_1$	$H3_121$

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell <i>P</i> or <i>R</i>			Triple cell <i>H</i>
		Short	Full	Extended	
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	$P3m1$		$P3m1$ <i>b</i>	$H31m$
157	C_{3v}^2	$P31m$		$P31m$ <i>a</i>	$H3m1$
158	C_{3v}^3	$P3c1$		$P3c1$ <i>n</i>	$H31c$
159	C_{3v}^4	$P31c$		$P31c$ <i>n</i>	$H3c1$
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	$\bar{P}31m$	$\bar{P}312/m$	$\bar{P}312/m$ $2_1/a$	$\bar{H}3m1$
163	D_{3d}^2	$\bar{P}31c$	$\bar{P}312/c$	$\bar{P}312/c$ $2_1/n$	$\bar{H}3c1$
164	D_{3d}^3	$\bar{P}3m1$	$\bar{P}32/m1$	$\bar{P}32/m1$ $2_1/b$	$\bar{H}31m$
165	D_{3d}^4	$\bar{P}3c1$	$\bar{P}32/c1$	$\bar{P}32/c1$ $2_1/n$	$\bar{H}31c$
166	D_{3d}^5	$\bar{R}3m$	$\bar{R}32/m$	$\bar{R}3\ 2/m$ $3_{1,2}2_1/b$	
167	D_{3d}^6	$\bar{R}3c$	$\bar{R}32/c$	$\bar{R}3\ 2/c$ $3_{1,2}2_1/n$	

HEXAGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell <i>P</i>			Triple cell <i>H</i>
		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	$\bar{P}6$			$\bar{H}6$
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	$H6_322$

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P			Triple cell H
		Short	Full	Extended	
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	$P\bar{6}2c$		$P\bar{6}2c$ 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	$P6_3/mmc$	$P6_3/m2/m2/c$	$P6_3/m$ $2/m$ $2/c$ $2_1/b$ $2_1/n$	$H6_3/mcm$

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	$Fm\bar{3}$	$F2/m\bar{3}$	$F2/m\bar{3}$ $2/n$ $2_1/b$ $2_1/a$
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	$Pa\bar{3}\ddagger$	$P2_1/a\bar{3}\ddagger$	
206	T_h^7	$Ia\bar{3}$	$I2_1/a\bar{3}$	$I2_1/a\bar{3}$ $2/b$
207	O^1	$P432$		$P432$ 2_1
208	O^2	$P4_232$		$P4_232$ 2_1

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols		
		Short	Full	Extended†
209	O^3	$F432$		$F432$ 42 $4_2 2_1$ $4_2 2_1$
210	O^4	$F4_1 32$		$F4_1 32$ $4_1 2$ $4_3 2_1$ $4_3 2_1$
211	O^5	$I432$		$I432$ $4_2 2_1$
212	O^6	$P4_3 32$		$P4_3 32$ 2_1
213	O^7	$P4_1 32$		$P4_1 32$ 2_1
214	O^8	$I4_1 32$		$I4_1 32$ $4_3 2_1$
215	T_d^1	$P\bar{4}3m$		$P\bar{4}3m$ g
216	T_d^2	$F\bar{4}3m$		$F\bar{4}3m$ g g_2 g_2
217	T_d^3	$I\bar{4}3m$		$I\bar{4}3m$ n
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	$Fm\bar{3}m$	$F4/m\bar{3}2/m$	$F4/m\bar{3}2/m$ $4/n 2/g$ $4_2/b 2_1/g_2$ $4_2/a 2_1/g_2$
226	O_h^6	$Fm\bar{3}c$	$F4/m\bar{3}2/c$	$F4/m\bar{3}2/n$ $4/n 2/c$ $4_2/b 2_1/g_1$ $4_2/a 2_1/g_1$
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	$Im\bar{3}m$	$I4/m\bar{3}2/m$	$I4/m\bar{3}2/m$ $4_2/n 2_1/n$
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. Section 1.5.4.1. ‡ The alternative setting $Pb\bar{3}$ ($P2_1/b\bar{3}$) of $Pa\bar{3}$ is of importance for diffraction studies, cf. Section 1.5.4.3 and Table 1.6.4.25. 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 $g_2(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$.

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

primitive lattice. In $Fmm2$ (42) for example, three additional lines appear in the extended symbol, namely $ba2$, $nc2_1$ and $cn2_1$. These operations are obtained by combining successively the centring translations $t(\frac{1}{2}, \frac{1}{2}, 0)$, $t(0, \frac{1}{2}, \frac{1}{2})$ and $t(\frac{1}{2}, 0, \frac{1}{2})$ with the symmetry operations of $Pmm2$. However, in space groups $Fdd2$ (43) and $Fddd$ (70) the nature of the d planes is not altered by the translations of the F -centred lattice; for this reason, in Table 1.5.4.4 a two-line symbol for $Fdd2$ and a one-line symbol for $Fddd$ are sufficient.

In tetragonal space groups with primitive lattices there are no alternating symmetry operations belonging to the symmetry directions [001] and [100]. However, for the symmetry direction $[1\bar{1}0]$ the symmetry operations 2 and 2_1 alternate, as do the reflection m and the glide reflection g [g is the name for a glide reflection with a glide vector $(\frac{1}{2}, \frac{1}{2}, 0)$], and the glide reflections c and n . For example, the second line of the extended symbol of $P4_2/n2/b2/c$ (133) contains the expression $2_1/n$ under the expression $2/c$.

For the space groups in the tetragonal system, the unique axis is always the c axis, thus reducing the number of settings and choices of the unit cell. Two additional multiple cells are considered in this system, namely the C and F cells obtained from the P and I cell by the following relations:

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b}; \quad \mathbf{b}' = \pm \mathbf{a} + \mathbf{b}; \quad \mathbf{c}' = \mathbf{c}.$$

The secondary [100] and tertiary [110] symmetry directions are interchanged in this cell transformation. As an example, consider $P4/n$ (85) and its description with respect to a C -centred basis. Under the transformation $\mathbf{a}' = \mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, the n glide $n(\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ is transformed to an a glide a $x, y, 0$ while its coplanar equivalent glide $n(-\frac{1}{2}, \frac{1}{2}, 0)$ $x, y, 0$ is transformed to a b glide b $x, y, 0$. Thus, the extended symbol of the multiple-cell description of $P4/n$ (85) shown in Table 1.5.4.4 is $C4/a(b)$, while in accordance with the e -glide convention, the short Hermann–Mauguin symbol becomes $C4/e$.

In the case of $I4/m$ (87), as a result of the I centring, screw rotations 4_2 and glide reflections n normal to 4_2 appear as additional symmetry operations and are shown in the second line of the extended symbol (cf. Table 1.5.4.4). In the multiple-cell setting, the space group $F4/m$ exhibits the additional fourfold screw axis 4_2 and owing to the new orientation of the a' and b' axes, which are rotated by 45° relative to the original axes a and b , the n glide of $I4/m$ becomes an a glide in the extended Hermann–Mauguin symbol. The additional b glide obtained from a coplanar n glide is not given explicitly in the extended symbol.

The rhombohedral space groups are listed together with the trigonal space groups under the heading ‘Trigonal system’. For both representative symmetry directions $[001]_{\text{hex}}$ and $[100]_{\text{hex}}$, rotations with screw rotations and reflections with glide reflections or different kinds of glide reflections alternate, so that additional symmetry operations always occur: rotations 3 or rotoinversions $\bar{3}$ are accompanied by 3_1 and 3_2 screw rotations; 2 rotations alternate with 2_1 screw rotations and m reflections or c glide reflections alternate with additional glide reflections. As examples, under the full Hermann–Mauguin symbol $R\bar{3}$ (146) one finds $3_{1,2}$ and in the line under $R\bar{3}2/c$ (167) one finds $3_{1,2}$ $2_1/n$.

The extended Hermann–Mauguin symbols for space groups of the hexagonal crystal system retain the symbol for the primary symmetry direction [001]. Along the secondary (100) and tertiary $(1\bar{1}0)$ symmetry directions every horizontal axis 2 is accompanied by a screw rotation 2_1 , while the reflections and glide reflections, or different types of glide reflections, alternate.

The list of hexagonal and trigonal space-group symbols is completed by a multiple H cell, which is three times the volume of the corresponding P cell. The unit-cell transformation is obtained from the relation

$$\mathbf{a}' = \mathbf{a} - \mathbf{b}; \quad \mathbf{b}' = \mathbf{a} + 2\mathbf{b}; \quad \mathbf{c}' = \mathbf{c}$$

with centring points at $0, 0, 0$; $\frac{2}{3}, \frac{1}{3}, 0$ and $\frac{1}{3}, \frac{2}{3}, 0$. The new vectors \mathbf{a}' and \mathbf{b}' are rotated by -30° in the ab plane with respect to the old vectors \mathbf{a} and \mathbf{b} . There are altogether six possible such multiple cells rotated by $\pm 30^\circ$, $\pm 90^\circ$ and $\pm 150^\circ$ (cf. Table 1.5.1.1 and Fig. 1.5.1.8).

The hexagonal lattice is frequently referred to the orthorhombic C -centred cell (cf. Table 1.5.1.1 and Fig. 1.5.1.7). The volume of this centred cell is twice the volume of the primitive hexagonal cell and its basis vectors are mutually perpendicular.

In general, the space groups of the cubic system do not yield any additional orientations and only the short, full and extended symbols are given. The only exception to this general rule is the group $Pa\bar{3}$ (205) with its alternative setting $Pb\bar{3}$, whose basis vectors \mathbf{a}' , \mathbf{b}' , \mathbf{c}' are related by a rotation of 90° in the ab plane to the basis vectors \mathbf{a} , \mathbf{b} , \mathbf{c} of $Pa\bar{3}$: $\mathbf{a}' = \mathbf{b}$, $\mathbf{b}' = -\mathbf{a}$, $\mathbf{c}' = \mathbf{c}$. The different general reflection conditions of $Pb\bar{3}$ in comparison to those of $Pa\bar{3}$ indicate its importance for diffraction studies (cf. Table 1.6.4.25). In some extended symbols of the cubic groups, we note the use of the g or g_i type of glide reflections as in, for example, $F\bar{4}3c$ (219). The g glide is a generic form of a glide plane which is different from the usual glide planes denoted by a , b , c , n , d or e . The symbols g , g_1 and g_2 indicate specific glide components and orientations that are specified in the *Note* to Table 1.5.4.4.

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