

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

1.5.4. Synoptic tables of plane and space groups²

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It is already clear from Section 1.5.3.1 that the Hermann–Mauguin symbols of a space group depend on the choice of the basis vectors. The purpose of this section is to give an overview of a large selection of possible alternative settings of space groups and their Hermann–Mauguin symbols covering most practical cases. In particular, the synoptic tables include two main types of information:

- (i) Space-group symbols for various settings and choices of the basis. The axis transformations involve permutations of axes conserving the shape of the cell and also transformations leading to different cell shapes and multiple cells.
- (ii) *Extended* Hermann–Mauguin space-group symbols in addition to the short and full symbols. The three types of symbols, short, full and extended, provide different levels of information about the symmetry elements and the related symmetry operations of the space group (*cf.* Section 1.2.3 for definitions and discussion of the concepts of symmetry element, geometric element, element set and defining symmetry operation). The short and full Hermann–Mauguin symbols only display information about a chosen set of generators for a space group from which all the elements of a space group can in principle be deduced (*cf.* Section 1.4.1.4 for a detailed treatment of short and full Hermann–Mauguin symbols). The multiplicity of the general position in each space group gives the number of symmetry operations *modulo* the lattice translations. As already discussed in Section 1.4.2.4, the combinations of this representative set of symmetry operations with lattice translations give rise to *additional symmetry operations* and *additional symmetry elements*, displayed in the symmetry-element diagrams. The additional symmetry operations are also reflected in the so-called *extended Hermann–Mauguin symbols*, which were introduced in *International Tables for X-ray Crystallography* Volume I (1952). They were systematically developed and tabulated by Bertaut for the first edition of Volume A of *International Tables for Crystallography (IT A)*, published in 1983. The background for the correct construction and interpretation of the extended Hermann–Mauguin symbols is presented in the following section.

1.5.4.1. Additional symmetry operations and symmetry elements

In order to interpret (or even determine) the extended symbol for a space group, one has to recall that all operations that belong to the same coset with respect to the translation subgroup have the same linear part, but that not all symmetry operations within a coset are operations of the same type. Furthermore, symmetry operations in one coset can belong to element sets of different symmetry elements.

1.5.4.1.1. Determining the type of a symmetry operation

In this section, a procedure for determining the types of symmetry operations and the corresponding symmetry elements is explained. It is a development of the method of geometrical interpretation discussed in Section 1.2.2.4. The procedure is based on the origin-shift transformations discussed in Sections 1.5.1 and 1.5.2, and provides an efficient way of analysing the

additional symmetry operations and symmetry elements. The key to the procedure is the decomposition of the translation part \mathbf{w} of a symmetry operation $W = (\mathbf{W}, \mathbf{w})$ into an *intrinsic translation part* \mathbf{w}_g , which is fixed by the linear part \mathbf{W} of W and thus parallel to the geometric element of W , and a *location part* \mathbf{w}_l , which is perpendicular to the intrinsic translation part. Note that the space fixed by \mathbf{W} and the space perpendicular to this fixed space are complementary, *i.e.* their dimensions add up to 3, therefore this decomposition is always possible.

As described in Section 1.2.2.4, the determination of the intrinsic translation part of a symmetry operation $W = (\mathbf{W}, \mathbf{w})$ with linear part \mathbf{W} of order k is based on the fact that the k th power of W must be a pure translation, *i.e.* $W^k = (\mathbf{I}, \mathbf{t})$ for some lattice translation \mathbf{t} . The *intrinsic translation part* of W is then defined as $\mathbf{w}_g = (1/k)\mathbf{t}$.

The difference $\mathbf{w}_l = \mathbf{w} - \mathbf{w}_g$ is perpendicular to \mathbf{w}_g and it is called the *location part* of \mathbf{w} . This terminology is justified by the following observation: As explained in detail in Sections 1.5.1.3 and 1.5.2.3, under an origin shift by \mathbf{p} , a column \mathbf{x} of point coordinates is transformed to

$$\mathbf{x}' = (\mathbf{I}, -\mathbf{p})\mathbf{x} = (\mathbf{I}, \mathbf{p})^{-1}\mathbf{x},$$

making in particular \mathbf{p} the new origin, and a matrix–column pair (\mathbf{W}, \mathbf{w}) is transformed to

$$(\mathbf{W}', \mathbf{w}') = (\mathbf{I}, \mathbf{p})^{-1}(\mathbf{W}, \mathbf{w})(\mathbf{I}, \mathbf{p}).$$

Applied to the symmetry operation $(\mathbf{W}, \mathbf{w}_l)$, known as the *reduced symmetry operation* in which the full translation part is replaced by the location part (thereby neglecting the intrinsic translation part), an origin shift by \mathbf{p} results in

$$\begin{aligned} (\mathbf{I}, \mathbf{p})^{-1}(\mathbf{W}, \mathbf{w}_l)(\mathbf{I}, \mathbf{p}) &= (\mathbf{I}, -\mathbf{p})(\mathbf{W}, \mathbf{w}_l)(\mathbf{I}, \mathbf{p}) \\ &= (\mathbf{W}, \mathbf{W}\mathbf{p} - \mathbf{p} + \mathbf{w}_l) \\ &= (\mathbf{W}, (\mathbf{W} - \mathbf{I})\mathbf{p} + \mathbf{w}_l). \end{aligned}$$

This means that if it is possible to find an origin shift \mathbf{p} such that $(\mathbf{I} - \mathbf{W})\mathbf{p} = \mathbf{w}_l$, then with respect to the new origin the reduced symmetry operation $(\mathbf{W}, \mathbf{w}_l)$ is transformed to (\mathbf{W}, \mathbf{o}) . But since the subspace perpendicular to the fixed space of \mathbf{W} clearly does not contain any vector fixed by \mathbf{W} , the restriction of $\mathbf{I} - \mathbf{W}$ to this subspace is an invertible linear transformation, and therefore for every location part \mathbf{w}_l there is indeed a suitable \mathbf{p} perpendicular to the fixed space of \mathbf{W} such that $(\mathbf{I} - \mathbf{W})\mathbf{p} = \mathbf{w}_l$.

The fact that an origin shift by \mathbf{p} transforms the translation part of the reduced symmetry operation $(\mathbf{W}, \mathbf{w}_l)$ to \mathbf{o} is equivalent to \mathbf{p} being a fixed point of $(\mathbf{W}, \mathbf{w}_l)$, which can also be seen directly because

$$(\mathbf{W}, \mathbf{w}_l)\mathbf{p} = \mathbf{W}\mathbf{p} + \mathbf{w}_l = \mathbf{W}\mathbf{p} + (\mathbf{I} - \mathbf{W})\mathbf{p} = \mathbf{p}.$$

Note that for one fixed point \mathbf{p} of the reduced symmetry operation $(\mathbf{W}, \mathbf{w}_l)$, the full *set of fixed points*, as defined in Section 1.2.4, is obtained by adding \mathbf{p} to the fixed vectors of \mathbf{W} , because for an arbitrary fixed point \mathbf{p}_F of $(\mathbf{W}, \mathbf{w}_l)$ one has $\mathbf{W}\mathbf{p}_F + \mathbf{w}_l = \mathbf{p}_F$ and since also $\mathbf{W}\mathbf{p} + \mathbf{w}_l = \mathbf{p}$ one finds $\mathbf{W}(\mathbf{p}_F - \mathbf{p}) = \mathbf{p}_F - \mathbf{p}$, *i.e.* the difference between two fixed points is a vector that is fixed by \mathbf{W} . In other words, the geometric element of $(\mathbf{W}, \mathbf{w}_l)$ is the space fixed by \mathbf{W} , translated such that it runs through \mathbf{p} .

Finally, in order to determine the symmetry element of the symmetry operation correctly, it may be necessary to reduce the intrinsic translation part \mathbf{w}_g by a lattice translation in the fixed space of \mathbf{W} .

² With Tables 1.5.4.1, 1.5.4.2, 1.5.4.3 and 1.5.4.4 by E. F. Bertaut.

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Summarizing, the types of symmetry operations $W = (\mathbf{W}, \mathbf{w})$ and their symmetry elements can be identified as follows:

- (i) Decompose the translation part \mathbf{w} as $\mathbf{w} = \mathbf{w}_g + \mathbf{w}_l$, where \mathbf{w}_g and \mathbf{w}_l are mutually perpendicular and the intrinsic translation part \mathbf{w}_g is fixed by the linear part \mathbf{W} of W .
- (ii) Determine a shift of origin \mathbf{p} such that $(\mathbf{I} - \mathbf{W})\mathbf{p} = \mathbf{w}_l$, i.e. such that \mathbf{p} is a fixed point of the reduced operation $(\mathbf{W}, \mathbf{w}_l)$.
- (iii) For the correct determination of the defining operation of the symmetry element it may be necessary to reduce the intrinsic translation part \mathbf{w}_g by a lattice translation in the fixed space of \mathbf{W} , thus yielding a coplanar or coaxial equivalent symmetry operation.

This analysis allows one to read off the types of the symmetry operations and of the corresponding symmetry elements that occur for the coset $\mathcal{T}W$ of W . The following two sections provide examples illustrating that in some cases the coset does not contain symmetry operations belonging to symmetry elements of different type, while in others it does.

1.5.4.1.2. Cosets without additional types of symmetry elements

In cases where the linear part \mathbf{W} of a symmetry operation W fixes only the origin, all elements in the coset are of the same type. This is due to the fact that the translation part \mathbf{w} is decomposed as $\mathbf{w}_g = \mathbf{o}$ and $\mathbf{w}_l = \mathbf{w}$. Since \mathbf{W} fixes only the origin, $\mathbf{I} - \mathbf{W}$ is invertible and a fixed point \mathbf{p} of the reduced operation $(\mathbf{W}, \mathbf{w}_l) = (\mathbf{W}, \mathbf{w})$ can be found, as $\mathbf{p} = (\mathbf{I} - \mathbf{W})^{-1}\mathbf{w}$. This situation occurs when W is an inversion or a three-, four- or sixfold rotoinversion. The element set of the symmetry element of an inversion consists only of this inversion; the element set of a rotoinversion consists of the rotoinversion W and its inverse W^{-1} (the latter belonging to a different coset). Therefore, in these cases each symmetry operation in the coset of W belongs to the element set of a different symmetry element (of the same type, namely an inversion centre or a rotoinversion axis).

Note that the above argument does not apply to twofold rotoinversions, since these are in fact reflections which fix a plane perpendicular to the rotoinversion axis and not only a single point. The following two examples illustrate that translations from a primitive lattice do not give rise to symmetry elements of different type in the cases of either a reflection or glide reflection with normal vector along one of the coordinate axes, or of a rotation or screw rotation with rotation axis along one of the coordinate axes.

Example 1

Let $W = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ be an n glide with normal vector along the c axis. For the composition of W with an integral translation $t(u_1, u_2, u_3)$ one obtains a symmetry operation W' with

translation part $\mathbf{w}' = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ u_3 \end{pmatrix}$. The decomposition of \mathbf{w}' into

the intrinsic translation part and the location part gives

$\mathbf{w}'_g = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ 0 \end{pmatrix}$ and $\mathbf{w}'_l = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$. This shows that the intrinsic

translation part is only changed by the lattice vector $\begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$

and hence W' is a coplanar equivalent of the symmetry operation $W'' = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + u_3$, which is an n glide with glide plane normal to the c axis and located at $z = u_3/2$. One concludes that W and W' belong to symmetry elements of the same type. The same conclusion would in fact remain true in the case of a C -centred lattice, since the composition of W with

the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ would simply result in the intrinsic translation part being changed by the centring translation.

Example 2

As an example of a rotation, let $W = \bar{y}, x, z$ be a fourfold rotation $4^+ 0, 0, z$ around the c axis. Composing W with the translation $t(u_1, u_2, u_3)$ results in the symmetry operation $W' = \bar{y} + u_1, x + u_2, z + u_3$ with intrinsic translation part $\mathbf{w}'_g = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$ and location part $\mathbf{w}'_l = \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$. Since we assume a primitive lattice, u_3 is an integer, hence W' is a coaxial equivalent of the symmetry operation $W'' = \bar{y} + u_1, x + u_2, z$, which has intrinsic translation part \mathbf{o} . To locate the geometric element of W' , one notes that for

$$\mathbf{W} = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

one has

$$(\mathbf{I} - \mathbf{W})\mathbf{p} = \mathbf{w}'_l \text{ for } \mathbf{p} = \begin{pmatrix} (u_1 - u_2)/2 \\ (u_1 + u_2)/2 \\ 0 \end{pmatrix}.$$

The symmetry operation W' therefore belongs to the symmetry element of a fourfold rotation with the line $(u_1 - u_2)/2, (u_1 + u_2)/2, z$ as geometric element. This analysis shows that all symmetry operations in the coset $\mathcal{T}W$ belong to the same type of symmetry element, since for each of these symmetry operations a coaxial equivalent can be found that has zero screw component.

1.5.4.1.3. Examples with additional types of symmetry elements

The examples given in the previous section illustrate that in the case of a translation vector perpendicular to the symmetry axis or symmetry plane of a symmetry operation, the intrinsic translation vector remains unchanged and only the location of the geometric element is altered. In particular, composition with such a translation vector results in symmetry operations and symmetry elements of the same type. On the other hand, composition with translations parallel to the symmetry axis or symmetry plane give rise to coaxial or coplanar equivalents, which also belong to the same symmetry element. Combining these two observations shows that for integral translations, only translations along a direction inclined to the symmetry axis or symmetry plane can give rise to additional symmetry elements. For these cases, the additional symmetry operations and their locations are summarized in Table 1.5.4.1.

In space groups with a centred lattice, the translation subgroup contains also translations with non-integral components, and these often give rise to symmetry operations and symmetry elements of different types in the same coset. An overview of additional symmetry operations and their locations that occur due to centring vectors is given in Table 1.5.4.2. In rhombohedral space groups all additional types of symmetry elements occur already as a result of combinations with integral lattice translations (*cf.* Table 1.5.4.1). For this reason, the rhombohedral centring R case is not included in Table 1.5.4.2.

In Section 1.4.2.4 the occurrence of glide reflections in a space group of type $P4mm$ (due to integral translations inclined to a

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Table 1.5.4.1

Additional symmetry operations and their locations if the translation vector \mathbf{t} is inclined to the symmetry axis or symmetry plane

The table is restricted to integral translations and thus is valid for primitive lattices and for integral translations in centred lattices (for centring translations see Table 1.5.4.2).

Symmetry operation at the origin		Translation vector \mathbf{t}	Additional symmetry operation			Representative plane and space groups (numbers)
Symbol	Location		Symbol	Screw or glide component	Location	
<i>Tetragonal, rhombohedral and cubic coordinate systems</i>						
2	$x, x, 0$	$1, 0, 0$ $0, 1, 0$	2_1	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x + \frac{1}{2}, 0$	$P422$ (89) $R32$ (155) $P432$ (207)
m	x, x, z	$1, 0, 0$ $0, 1, 0$	g	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x + \frac{1}{2}, z$	$P4mm$ (11) $P4mm$ (99) $R3m$ (160) $P\bar{4}3m$ (215)
c	x, x, z	$1, 0, 0$ $0, 1, 0$	n	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x, x + \frac{1}{2}, z$	$P\bar{4}2c$ (112) $R3c$ (161) $P\bar{4}3n$ (218)
<i>Hexagonal coordinate system</i>						
2	$x, 0, 0$	$1, 1, 0$ $0, 1, 0$	2_1	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, 0$	$P321$ (150) $R32$ (155)
2	$x, 2x, 0$	$0, 1, 0$ $1, 1, 0$	2_1	$\frac{1}{2}, 1, 0$	$x, 2x + \frac{1}{2}, 0$	$P312$ (149) $P622$ (177)
m	$x, 2x, z$	$0, 1, 0$ $1, 1, 0$	b	$\frac{1}{2}, 1, 0$	$x, 2x + \frac{1}{2}, z$	$P3m1$ (156) $p3m1$ (14) $R3m$ (160)
c	$x, 2x, z$	$0, 1, 0$ $1, 1, 0$	n	$\frac{1}{2}, 1, \frac{1}{2}$	$x, 2x + \frac{1}{2}, z$	$P3c1$ (158) $P\bar{6}c2$ (188) $R3c$ (161)
m	$x, 0, z$	$1, 1, 0$ $0, 1, 0$	a	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, z$	$P31m$ (157) $p31m$ (15)
c	$x, 0, z$	$1, 1, 0$ $0, 1, 0$	n	$\frac{1}{2}, 0, \frac{1}{2}$ $-\frac{1}{2}, 0, \frac{1}{2}$	$x, \frac{1}{2}, z$	$P31c$ (159) $P\bar{6}2c$ (190)
<i>Rhombohedral and cubic coordinate systems</i>						
3	x, x, x	$1, 0, 0$ $0, 1, 0$ $0, 0, 1$	3_1	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	$x, x + \frac{2}{3}, x + \frac{1}{3}$	$R3$ (146) $P23$ (195)
3	x, x, x	$2, 0, 0$ $0, 2, 0$ $0, 0, 2$	3_2	$\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$	$x, x + \frac{1}{3}, x + \frac{2}{3}$	

symmetry plane) and of type $Fmm2$ (due to centring translations) is discussed. We now provide some further examples illustrating the contents of Tables 1.5.4.1 and 1.5.4.2.

Example 3

Let $W = z, x, y$ be a threefold rotation 3^+ x, x, x along the [111] direction in a cubic (or rhombohedral) space group. Then the coset TW also contains the symmetry operation $W' = z + 1, x, y$. With

$$W = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

one sees that $(W')^3 = t(1, 1, 1)$ and hence the intrinsic translation part is

$$w'_g = \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix}.$$

It follows that the location part is $w'_l = \begin{pmatrix} \frac{2}{3} \\ -\frac{1}{3} \\ -\frac{1}{3} \end{pmatrix}$ and one finds that $(I - W)p = w'_l$ for $p = \begin{pmatrix} \frac{2}{3} \\ \frac{1}{3} \\ 0 \end{pmatrix}$. Thus, the symmetry

operation $W' = z + 1, x, y$ is of a different type to W : it is a threefold screw rotation $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x + \frac{2}{3}, x + \frac{1}{3}, x$ with the line $x + \frac{2}{3}, x + \frac{1}{3}, x$ as geometric element.

On the other hand, for an integer $u \neq 0$, the symmetry operation $W'' = z + u, x + u, y + u$ itself is a screw rotation, but it belongs to a symmetry element of rotation type, since it is a coaxial equivalent of the threefold rotation W . The crucial difference between the symmetry operations $W' = z + 1, x, y$ and $W'' = z + u, x + u, y + u$ is that in the latter case the

intrinsic translation part $\begin{pmatrix} u \\ u \\ u \end{pmatrix}$ is a lattice vector, whereas for $W' = z + 1, x, y$ it is not.

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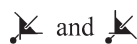
Table 1.5.4.2

Additional symmetry operations due to a centring vector \mathbf{t} and their locations

Symmetry operation at the origin		Additional symmetry operations									Representative space groups (numbers)	
Symbol	Location	$C, t(\frac{1}{2}, \frac{1}{2}, 0)$		$A, t(0, \frac{1}{2}, \frac{1}{2})$		$B, t(\frac{1}{2}, 0, \frac{1}{2})$		$I, t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		F		
m	$0, y, z$	b	$\frac{1}{4}, y, z$	n	$0, y, z$	c	$\frac{1}{4}, y, z$	n	$\frac{1}{4}, y, z$	b, n, c	<i>Cmmm, Ammm, Bmmm</i> (65) <i>Immm</i> (71), <i>Fmmm</i> (69) <i>Cccm, Amaa, Bbmb</i> (66), <i>Ibca</i> (73) <i>Fddd</i> (70)	
c		n		b		m		b				
b		m		c		n		c				
$d(0, \frac{1}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{3}{4})$		$d(0, \frac{1}{4}, \frac{3}{4})$				d, d, d		
m	$x, 0, z$	a	$x, \frac{1}{4}, z$	c	$x, \frac{1}{4}, z$	n	$x, 0, z$	n	$x, \frac{1}{4}, z$	a, c, n	As above	
a		m		n		c		c				
c		n		m		a		a				
$d(\frac{1}{4}, 0, \frac{1}{4})$		$d(\frac{3}{4}, 0, \frac{1}{4})$		$d(\frac{1}{4}, 0, \frac{3}{4})$		$d(\frac{3}{4}, 0, \frac{3}{4})$				d, d, d		
m	$x, y, 0$	n	$x, y, 0$	b	$x, y, \frac{1}{4}$	a	$x, y, \frac{1}{4}$	n	$x, y, \frac{1}{4}$	n, b, a	As above	
b		a		m		n		a				
a		b		n		m		b				
$d(\frac{1}{4}, \frac{1}{4}, 0)$		$d(\frac{3}{4}, \frac{3}{4}, 0)$		$d(\frac{1}{4}, \frac{3}{4}, 0)$		$d(\frac{3}{4}, \frac{1}{4}, 0)$				d, d, d		
m	x, x, z	$g(\frac{1}{2}, \frac{1}{2}, 0)$	x, x, z	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x + \frac{1}{4}, z$	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x - \frac{1}{4}, z$	$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	x, x, z	g, g, g	<i>I4mm</i> (107), <i>F43m</i> (216)	
c		$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{2}, \frac{1}{2}, 0)$		n, g, g		<i>F43c</i> (219)
$d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$								$d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$				<i>I43d</i> (220)
2	$x, 0, 0$	2_1	$x, \frac{1}{4}, 0$	2	$x, \frac{1}{4}, \frac{1}{4}$	2_1	$x, 0, \frac{1}{4}$	2_1	$x, \frac{1}{4}, \frac{1}{4}$	$2_1, 2, 2_1$	<i>C222, A222, B222</i> (21) <i>I222</i> (23) <i>F222</i> (22) <i>C422 (P422)</i> (89), <i>I422</i> (97) <i>F432</i> (209) <i>F4132</i> (210) <i>Immm</i> (71), <i>Fmmm</i> (69)	
2	$0, y, 0$	2_1	$\frac{1}{4}, y, 0$	2_1	$0, y, \frac{1}{4}$	2	$\frac{1}{4}, y, \frac{1}{4}$	2_1	$\frac{1}{4}, y, \frac{1}{4}$	$2_1, 2_1, 2$		
2	$0, 0, z$	2	$\frac{1}{4}, \frac{1}{4}, z$	2_1	$0, \frac{1}{4}, z$	2_1	$\frac{1}{4}, 0, z$	2_1	$\frac{1}{4}, \frac{1}{4}, z$	$2, 2_1, 2_1$		
2	$x, \bar{x}, 0$	2	$x, \bar{x} + \frac{1}{2}, 0$	$2_1(-\frac{1}{4}, \frac{1}{4}, 0)$	$x, \bar{x} + \frac{1}{4}, \frac{1}{4}$	$2_1(\frac{1}{4}, -\frac{1}{4}, 0)$	$x, \bar{x} + \frac{1}{4}, \frac{1}{4}$	2	$x, \bar{x}, \frac{1}{4}$	$2, 2_1, 2_1$		
4	$0, 0, z$	4	$0, \frac{1}{2}, z$	4_2	$-\frac{1}{4}, \frac{1}{4}, z$	4_2	$\frac{1}{4}, \frac{1}{4}, z$	4_2	$0, \frac{1}{2}, z$	$4, 4_2, 4_2$		
4_1	$0, 0, z$	4_1	$0, \frac{1}{2}, z$	4_3	$-\frac{1}{4}, \frac{1}{4}, z$	4_3	$\frac{1}{4}, \frac{1}{4}, z$	4_3	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$		
$\bar{1}$	$0, 0, 0$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\bar{1}, \bar{1}, \bar{1}$		

This example illustrates in particular the occurrence of symmetry elements of screw or glide type even in the case of symmorphic space groups where all coset representatives $W = (W, \mathbf{w})$ with respect to the translation subgroup can be chosen with $\mathbf{w} = \mathbf{o}$.

Note that, mainly for historical reasons, the screw rotations resulting from the threefold rotation along the [111] direction are not included in the extended Hermann–Mauguin symbol of cubic space groups, cf. Table 1.5.4.4. However, these screw rotations are represented in the cubic symmetry-element diagrams by the symbols



(cf. Table 2.1.2.7), as can be observed in the symmetry-element diagram for a group of type $P23$ (195) in Fig. 1.5.4.1.

Example 4

A twofold rotation $W = y, x, \bar{z}$ with the line $x, x, 0$ as geometric element has linear part

$$W = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}.$$

The composition W' of W with the translation $t(0, 1, 0)$ has

intrinsic translation part $\mathbf{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\mathbf{w}'_l = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$. Since $(I - W)\mathbf{p} = \mathbf{w}'_l$ for $\mathbf{p} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$, the

symmetry operation $W' = y, x + \frac{1}{2}, \bar{z}$ is a screw rotation $2(\frac{1}{2}, \frac{1}{2}, 0)x, x + \frac{1}{2}, 0$ with the line $x, x + \frac{1}{2}, 0$ as geometric element and is thus of a different type to W (cf. Table 1.5.4.1).

In an I -centred lattice, the composition of W with the centring translation $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ has intrinsic translation part $\mathbf{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\mathbf{w}'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$. One has $(I - W)\mathbf{p} = \mathbf{w}'_l$ for $\mathbf{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, hence the symmetry operation $W' = y + \frac{1}{2}, x + \frac{1}{2}, \bar{z} + \frac{1}{2}$ is a screw rotation $2(\frac{1}{2}, \frac{1}{2}, 0)x, x, \frac{1}{4}$ with the line $x, x, \frac{1}{4}$ as geometric element and is thus of a different type to W .

On the other hand, the translation subgroup T also contains the translation $t(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})$. In this case, the intrinsic translation part of $W' = y + \frac{1}{2}, x - \frac{1}{2}, \bar{z} + \frac{1}{2}$ is $\mathbf{w}'_g = \mathbf{o}$, hence W' is of the same type as W , i.e. a twofold rotation. The location part is

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

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

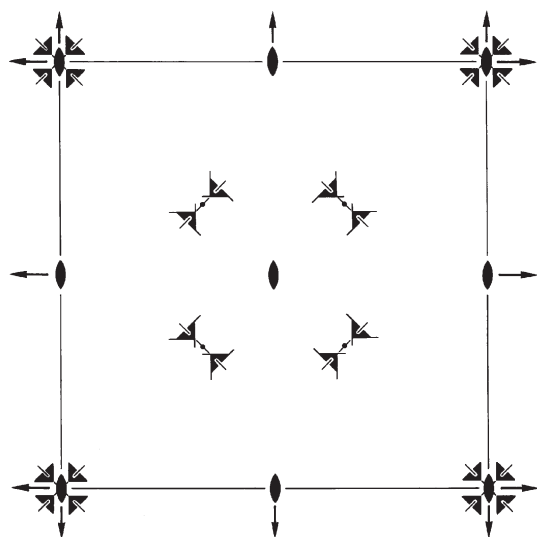


Figure 1.5.4.1
Symmetry-element diagram for space group $P23$ (195).

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>p6mm</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)

1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

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	2_1	2_1	2_1	2_1	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	Cell choice 3
			$I1m1$	$I1m1$	$I11m$	$I11m$	$Im11$	$Im11$	
9	C_s^4	Cc	n	n	n	n	n	n	Cell choice 1
			$C1c1$	$A1a1$	$A11a$	$B11b$	$Bb11$	$Cc11$	Cell choice 2
			n	n	n	n	n	n	Cell choice 3
			$A1n1$	$C1n1$	$B11n$	$A11n$	$Cn11$	$Bn11$	
			a	c	b	a	c	b	Cell choice 1
			$I1a1$	$I1c1$	$I11b$	$I11a$	$Ic11$	$Ib11$	Cell choice 2
			c	a	a	b	b	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	$C2/m$	$C1\frac{2}{m}1$	$A1\frac{2}{m}1$	$A11\frac{2}{m}$	$B11\frac{2}{m}$	$B\frac{2}{m}11$	$C\frac{2}{m}11$	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}	\overline{cba}	\underline{abc}	$\underline{ba\bar{c}}$	\underline{abc}	\overline{acb}	
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}	\overline{cba}	\underline{bca}	$\overline{a\bar{c}b}$
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> 2 ₁ <i>cn</i>	<i>A</i> 2 ₁ <i>am</i> 2 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> 2 ₁ <i>nn</i>	<i>A</i> 2 ₁ <i>aa</i> 2 ₁ <i>nn</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> 2 ₁ <i>na</i>	<i>C</i> 2 ₁ <i>mm</i> 2 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>) 2 ₁ <i>aa</i>	<i>C</i> 2 ₁ <i>mb</i> (<i>C2me</i>) 2 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> 2 ₁ <i>nn</i>	<i>C</i> 2 ₁ <i>cm</i> 2 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>) 2 ₁ <i>an</i>	<i>C</i> 2 ₁ <i>cb</i> (<i>C2ce</i>) 2 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> 2 ₁ <i>cb</i> 2 ₁ <i>na</i> 2 ₁ <i>an</i>	<i>F</i> 2 ₁ <i>mm</i> 2 ₁ <i>cb</i> 2 ₁ <i>an</i> 2 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> 2 ₁ <i>dd</i>	<i>F</i> 2 ₁ <i>dd</i> 2 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> 2 ₁ <i>nn</i>	<i>I</i> 2 ₁ <i>mm</i> 2 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> 2 ₁ <i>aa</i>	<i>I</i> 2 ₁ <i>cb</i> 2 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> 2 ₁ <i>na</i>	<i>I</i> 2 ₁ <i>cm</i> 2 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	$P4mm$	$P4mm$ <i>g</i>	$C4mm$	$C4mm$ <i>b</i>
100	C_{4v}^2	$P4bm$	$P4bm$ <i>g</i>	$C4mg_1$	$C4mg_1$ <i>b</i>
101	C_{4v}^3	$P4_2cm$	$P4_2cm$ <i>g</i>	$C4_2mc$	$C4_2mc$ <i>b</i>
102	C_{4v}^4	$P4_2nm$	$P4_2nm$ <i>g</i>	$C4_2mg_2$	$C4_2mg_2$ <i>b</i>
103	C_{4v}^5	$P4cc$	$P4cc$ <i>n</i>	$C4cc$	$C4cc$ <i>n</i>
104	C_{4v}^6	$P4nc$	$P4nc$ <i>n</i>	$C4cg_2$	$C4cg_2$ <i>n</i>
105	C_{4v}^7	$P4_2mc$	$P4_2mc$ <i>n</i>	$C4_2cm$	$C4_2cm$ <i>n</i>
106	C_{4v}^8	$P4_2bc$	$P4_2bc$ <i>n</i>	$C4_2cg_1$	$C4_2cg_1$ <i>n</i>
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	$P\bar{4}2m$	$P\bar{4}2m$ <i>g</i>	$C\bar{4}m2$	$C\bar{4}m2$ <i>b</i>
112	D_{2d}^2	$P\bar{4}2c$	$P\bar{4}2c$ <i>n</i>	$C\bar{4}c2$	$C\bar{4}c2$ <i>n</i>
113	D_{2d}^3	$P\bar{4}2_1m$	$P\bar{4}2_1m$ <i>g</i>	$C\bar{4}m2_1$	$C\bar{4}m2_1$ <i>b</i>
114	D_{2d}^4	$P\bar{4}2_1c$	$P\bar{4}2_1c$ <i>n</i>	$C\bar{4}c2_1$	$C\bar{4}c2_1$ <i>n</i>
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	$P4/mbm$	$P4/m\ 2_1/b\ 2/m\ 2_1/g$	$C4/mmg_1$	$C4/mng_1\ nb$
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	$P3_12$		$P3_12\ 2_1$	$H3_121$

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 $R3$ (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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