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1.5.4. Synoptic tables of plane and space groups[2]

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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 $\boldsymbol{w}$ of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ into an *intrinsic translation part* $\boldsymbol{w}_g$, which is fixed by the linear part $\boldsymbol{W}$ of W and thus parallel to the geometric element of W, and a *location part* $\boldsymbol{w}_l$, which is perpendicular to the intrinsic translation part. Note that the space fixed by $\boldsymbol{W}$ 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 $W = (\boldsymbol{W}, \boldsymbol{w})$ with linear part $\boldsymbol{W}$ of order k is based on the fact that the kth power of W must be a pure translation, *i.e.* $W^k = (\boldsymbol{I}, \boldsymbol{t})$ for some lattice translation $\boldsymbol{t}$. The *intrinsic translation part* of W is then defined as $\boldsymbol{w}_g = (1/k)\boldsymbol{t}$.

The difference $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{w}_g$ is perpendicular to $\boldsymbol{w}_g$ and it is called the *location part* of $\boldsymbol{w}$. 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 $\boldsymbol{p}$, a column $\boldsymbol{x}$ of point coordinates is transformed to

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

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

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

Applied to the symmetry operation $(\boldsymbol{W}, \boldsymbol{w}_l)$, 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 $\boldsymbol{p}$ results in

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

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

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

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

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

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

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

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

(i) Decompose the translation part $\boldsymbol{w}$ as $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$, where $\boldsymbol{w}_g$ and $\boldsymbol{w}_l$ are mutually perpendicular and the intrinsic translation part $\boldsymbol{w}_g$ is fixed by the linear part $\boldsymbol{W}$ of $\mathcal{W}$.

(ii) Determine a shift of origin $\boldsymbol{p}$ such that $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}_l$, *i.e.* such that $\boldsymbol{p}$ is a fixed point of the reduced operation $(\boldsymbol{W}, \boldsymbol{w}_l)$.

(iii) For the correct determination of the defining operation of the symmetry element it may be necessary to reduce the intrinsic translation part $\boldsymbol{w}_g$ by a lattice translation in the fixed space of $\boldsymbol{W}$, 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 $\mathcal{T}\mathcal{W}$ of $\mathcal{W}$. 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 $\boldsymbol{W}$ of a symmetry operation $\mathcal{W}$ fixes only the origin, all elements in the coset are of the same type. This is due to the fact that the translation part $\boldsymbol{w}$ is decomposed as $\boldsymbol{w}_g = \boldsymbol{o}$ and $\boldsymbol{w}_l = \boldsymbol{w}$. Since $\boldsymbol{W}$ fixes only the origin, $\boldsymbol{I} - \boldsymbol{W}$ is invertible and a fixed point $\boldsymbol{p}$ of the reduced operation $(\boldsymbol{W}, \boldsymbol{w}_l) = (\boldsymbol{W}, \boldsymbol{w})$ can be found, as $\boldsymbol{p} = (\boldsymbol{I} - \boldsymbol{W})^{-1}\boldsymbol{w}$. This situation occurs when $\mathcal{W}$ 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 $\mathcal{W}$ and its inverse $\mathcal{W}^{-1}$ (the latter belonging to a different coset). Therefore, in these cases each symmetry operation in the coset of $\mathcal{W}$ 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 $\mathcal{W} = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ be an n glide with normal vector along the c axis. For the composition of $\mathcal{W}$ with an integral translation $t(u_1, u_2, u_3)$ one obtains a symmetry operation $\mathcal{W}'$ with translation part $\boldsymbol{w}' = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ u_3 \end{pmatrix}$. The decomposition of $\boldsymbol{w}'$ into the intrinsic translation part and the location part gives $\boldsymbol{w}'_g = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ 0 \end{pmatrix}$ and $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$. 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 $\mathcal{W}'$ is a coplanar equivalent of the symmetry operation $\mathcal{W}'' = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + u_3$, which is an n glide with glide plane normal to the c axis and located at $z = u_3/2$. One concludes that $\mathcal{W}$ and $\mathcal{W}'$ 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 $\mathcal{W}$ 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 $\mathcal{W} = \bar{y}, x, z$ be a fourfold rotation $4^+\ 0, 0, z$ around the c axis. Composing $\mathcal{W}$ with the translation $t(u_1, u_2, u_3)$ results in the symmetry operation $\mathcal{W}' = \bar{y} + u_1, x + u_2, z + u_3$ with intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$. Since we assume a primitive lattice, u_3 is an integer, hence $\mathcal{W}'$ is a coaxial equivalent of the symmetry operation $\mathcal{W}'' = \bar{y} + u_1, x + u_2, z$, which has intrinsic translation part $\boldsymbol{o}$. To locate the geometric element of $\mathcal{W}'$, one notes that for

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

one has

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

The symmetry operation $\mathcal{W}'$ 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 $\mathcal{T}\mathcal{W}$ 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

Table 1.5.4.1
Additional symmetry operations and their locations if the translation vector **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			Additional symmetry operation			Representative plane and space groups (numbers)
Symbol	Location	Translation vector **t**	Symbol	Screw or glide component	Location	
Tetragonal, rhombohedral and cubic coordinate systems						
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)
Hexagonal coordinate system						
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)
Rhombohedral and cubic coordinate systems						
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 $\mathcal{T}W$ also contains the symmetry operation $W' = z+1, x, y$. With

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

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

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

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

Table 1.5.4.2
Additional symmetry operations due to a centring vector **t** and their locations

Symmetry operation at the origin		Additional symmetry operations									Representative space groups (numbers)
		$C, t(\frac{1}{2},\frac{1}{2},0)$		$A, t(0,\frac{1}{2},\frac{1}{2})$		$B, t(\frac{1}{2},0,\frac{1}{2})$		$I, t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$		F	
Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	
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	*Cmmm*, *Ammm*, *Bmmm* (65)
c		n		b		m		b			*Immm* (71), *Fmmm* (69)
b		m		c		n		c			*Cccm*, *Amaa*, *Bbmb* (66), *Ibca* (73)
$d(0,\frac{1}{4},\frac{1}{4})$		$d(0,\frac{3}{4},\frac{1}{4})$		$d(0,\frac{3}{4},\frac{3}{4})$		$d(0,\frac{1}{4},\frac{3}{4})$				d, d, d	*Fddd* (70)
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*4*mm* (107), $F\bar{4}3m$ (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	$F\bar{4}3c$ (219)
$d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$								$d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$			$I\bar{4}3d$ (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	$x, \frac{1}{4}, \frac{1}{4}$	$2_1, 2, 2_1$	*C*222, *A*222, *B*222 (21)
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	$\frac{1}{4}, y, \frac{1}{4}$	$2_1, 2_1, 2$	*I*222 (23)
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	$\frac{1}{4}, \frac{1}{4}, z$	$2, 2_1, 2_1$	*F*222 (22)
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	$x, \bar{x}, \frac{1}{4}$	$2, 2_1, 2_1$	*C*422 (*P*422) (89), *I*422 (97)
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	$0, \frac{1}{2}, z$	$4, 4_2, 4_2$	*F*432 (209)
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	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$	$F4_132$ (210)
$\bar{1}$	$0, 0, 0$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\bar{1}, \bar{1}, \bar{1}$	*Immm* (71), *Fmmm* (69)

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 $W = (\boldsymbol{W}, \boldsymbol{w})$ with respect to the translation subgroup can be chosen with $\boldsymbol{w} = \boldsymbol{o}$.

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

 and 

(*cf.* Table 2.1.2.7), as can be observed in the symmetry-element diagram for a group of type *P*23 (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

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

The composition W' of W with the translation $t(0, 1, 0)$ has intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$. Since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$, 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 $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$. One has $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, 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 $\mathcal{T}$ 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 $\boldsymbol{w}'_g = \boldsymbol{o}$, hence W' is of the same type as W, *i.e.* a twofold rotation. The location part is $\boldsymbol{w}'_l = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$ and since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{4} \end{pmatrix}$, the geometric element of W' is the line $x + \frac{1}{2}, x, \frac{1}{4}$.

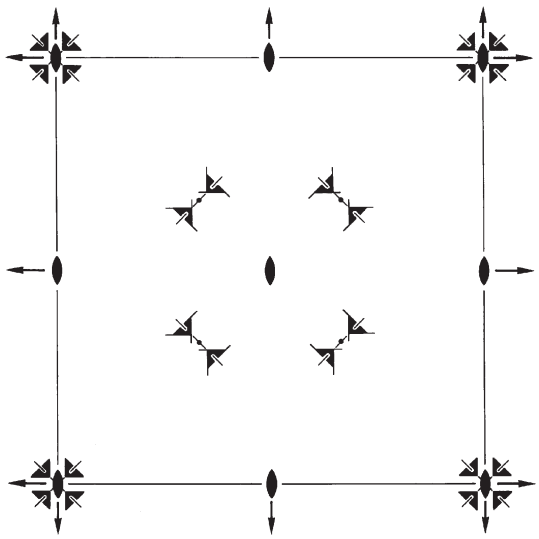

Figure 1.5.4.1
Symmetry-element diagram for space group $P23$ (195).

The analysis illustrates that the combination of the twofold rotation $2\ x, x, 0$ 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 $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and consequently the location part is $\boldsymbol{w}'_l = \boldsymbol{o}$. The symmetry operation W' is thus an n glide with the plane $x, y, 0$ as geometric element. However, since the intrinsic translation part $\boldsymbol{w}_g$ 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 $\boldsymbol{w}'_g = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$. The location part is $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$ and since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, 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

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

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

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

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 $P\bar{1}$ (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 $\mathbf{a}\underline{\mathbf{b}}\mathbf{c}$ and $\mathbf{c}\underline{\bar{\mathbf{b}}}\mathbf{a}$, $\mathbf{a}\mathbf{b}\underline{\mathbf{c}}$ and $\mathbf{b}\mathbf{a}\underline{\bar{\mathbf{c}}}$, $\underline{\mathbf{a}}\mathbf{b}\mathbf{c}$ and $\underline{\bar{\mathbf{a}}}\mathbf{c}\mathbf{b}$. 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 centrings give 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.