1.5. Transformations of coordinate systems

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It is in general advantageous to refer crystallographic objects and their symmetries to the most appropriate coordinate system. The best coordinate system may be different for different steps of the calculations and for different objects which have to be considered simultaneously. Therefore, a change of the origin and/or the basis are frequently necessary when treating crystallographic problems, for example in the study of phase-transition phenomena, or in the comparison of crystal structures described with respect to different coordinate systems.

1.5.1. Origin shift and change of the basis[1]

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1.5.1.1. Origin shift

Let a coordinate system be given with a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and an origin O. Referred to this coordinate system, the column of coordinates of a point X is $\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ and the corresponding vector is $\mathbf{x} = x_1\mathbf{a} + x_2\mathbf{b} + x_3\mathbf{c}$. Referred to a new coordinate system, specified by the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and the origin O', the column of coordinates of the point X is $\boldsymbol{x}' = \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix}$. Let $\boldsymbol{p} = \overrightarrow{OO'} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$ be the column of coefficients for the vector $\mathbf{p}$ from the old origin O to the new origin O', see Fig. 1.5.1.1.

For the columns $\boldsymbol{p} + \boldsymbol{x}' = \boldsymbol{x}$ holds, *i.e.*

$$\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{p} \quad \text{or} \quad \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} x_1 - p_1 \\ x_2 - p_2 \\ x_3 - p_3 \end{pmatrix}. \tag{1.5.1.1}$$

This can be written in the formalism of matrix–column pairs (*cf.* Section 1.2.2.3 for details of the matrix–column formalism) as

$$\boldsymbol{x}' = (\boldsymbol{I}, -\boldsymbol{p})\boldsymbol{x} \quad \text{or} \quad \boldsymbol{x}' = (\boldsymbol{I}, \boldsymbol{p})^{-1}\boldsymbol{x}, \tag{1.5.1.2}$$

where $(\boldsymbol{I}, \boldsymbol{p})$ represents the translation corresponding to the vector $\mathbf{p}$ of the origin shift.

The vector $\mathbf{r}$ determined by the points X and Y (also known as a 'distance vector'), $\mathbf{x} + \mathbf{r} = \mathbf{y}$ (*cf.* Fig. 1.5.1.1), and thus with coefficients

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix},$$

shows a different transformation behaviour under the origin shift. From the diagram one reads the equations $\mathbf{p} + \mathbf{x}' = \mathbf{x}$, $\mathbf{x} + \mathbf{r} = \mathbf{y}$, $\mathbf{x}' + \mathbf{r} = \mathbf{y}'$, and thus

$$\mathbf{r} = \mathbf{y}' - \mathbf{x}' = \mathbf{y} - \mathbf{x}, \tag{1.5.1.3}$$

i.e. the vector coefficients of $\mathbf{r}$ are not affected by the origin shift.

Example

The description of a crystal structure is closely related to its space-group symmetry: different descriptions of the underlying space group, in general, result in different descriptions of the crystal structure. This example illustrates the comparison of two structure descriptions corresponding to different origin choices of the space group.

To compare the two structures it is not only necessary to apply the origin-shift transformation but also to adjust the selection of the representative atoms of the two descriptions.

In the Inorganic Crystal Structure Database (2012) (abbreviated as ICSD) one finds the following two descriptions of the mineral zircon $ZrSiO_4$:

(*a*) Wyckoff & Hendricks (1927), ICSD No. 31101, space group $I4_1/amd = D_{4h}^{19}$, No. 141, cell parameters a = 6.61 Å, c = 5.98 Å.

The coordinates of the atoms in the unit cell are (normalized so that $0 \le x_i < 1$):

Zr:	4*a*	0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{4}$ [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+]
Si:	4*b*	0, 0, $\frac{1}{2}$; 0, $\frac{1}{2}$, $\frac{3}{4}$ [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+]
O:	16*h*	0, 0.2, 0.34; 0.5, 0.3, 0.84; 0.8, 0.5, 0.59; 0.7, 0, 0.09; 0.5, 0.2, 0.41; 0, 0.3, 0.91; 0.7, 0.5, 0.16; 0.8, 0, 0.66 [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+].

The coordinates of Zr and Si atoms indicate that the space-group setting corresponds to the origin choice 1 description of $I4_1/amd$ given in this volume, *i.e.* origin at $\bar{4}m2$ (*cf.* the space-group tables for $I4_1/amd$ in Chapter 2.3).

(*b*) Krstanovic (1958), ICSD No. 45520, space group $I4_1/amd = D_{4h}^{19}$, No. 141, cell parameters a = 6.6164 (5) Å, c = 6.0150 (5) Å.

The coordinates of the atoms in the unit cell are (normalized so that $0 \le x_i < 1$):

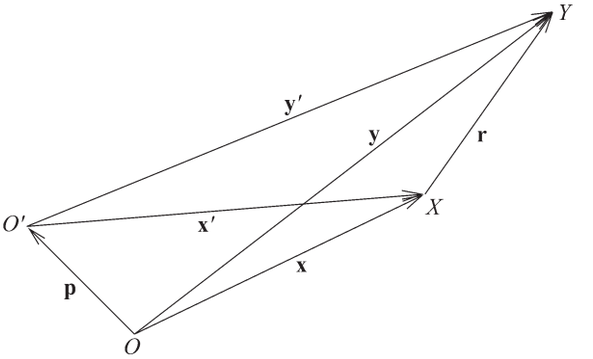


Figure 1.5.1.1
The coordinates of the points X (or Y) with respect to the old origin O are $\boldsymbol{x}$ ($\boldsymbol{y}$), and with respect to the new origin O' they are $\boldsymbol{x}'$ ($\boldsymbol{y}'$). From the diagram one reads $\mathbf{p} + \mathbf{x}' = \mathbf{x}$ and $\mathbf{p} + \mathbf{y}' = \mathbf{y}$.

[1] With Table 1.5.1.1 and Figs. 1.5.1.2 and 1.5.1.5–1.5.1.10 by H. Arnold.

Zr:	4*a*	$0, \frac{3}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$ [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$]
Si:	4*b*	$0, \frac{1}{4}, \frac{3}{8}$; $0, \frac{3}{4}, \frac{5}{8}$ [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$]
O:	16*h*	0, 0.067, 0.198; 0.5, 0.933, 0.698; 0.183, 0.75, 0.448; 0.317, 0.25, 0.948; 0.5, 0.067, 0.302; 0, 0.933, 0.802; 0.317, 0.75, 0.052; 0.183, 0.25, 0.552 [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$].

The structure is described with respect to the origin choice 2 setting of $I4_1/amd$ specified in this volume as 'Origin at centre $(2/m)$ at $0, \frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$' (*cf.* the space-group tables for $I4_1/amd$ in Chapter 2.3).

In order to compare the different structure descriptions, the atomic coordinates of the origin choice 1 description are to be transformed to 'Origin at centre $2/m$', *i.e.* origin choice 2.

Origin choice 2 has coordinates $0, \frac{1}{4}, \frac{1}{8}$ referred to origin choice 1. Therefore, the change of coordinates consists of *subtracting* $\boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{4} \\ \frac{1}{8} \end{pmatrix}$ from the origin choice 1 values, *i.e.* leave the x coordinate unchanged, add $\frac{1}{4} = 0.25$ to the y coordinate and subtract $\frac{1}{8} = 0.125$ from the z coordinate [*cf.* equation (1.5.1.1)].

The transformed and normalized coordinates (so that $0 \leq x_i < 1$) are

(i) Zr: 4*a* $0, \frac{1}{4}, \frac{7}{8}$; $0, \frac{3}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{1}{4}, \frac{5}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$;

(ii) Si: 4*b* $0, \frac{1}{4}, \frac{3}{8}$; $0, \frac{3}{4}, \frac{5}{8}$; $\frac{1}{2}, \frac{1}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{7}{8}$;

(iii) O: 16*h* $0, 0.20 + 0.25, 0.34 - 0.125 = 0, 0.45, 0.215$.

This oxygen atom obviously does not correspond to the representative 0, 0.067, 0.198 given by Krstanovic (1958), but by adding the centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ it is seen to correspond to the second position with coordinates 0.5, 0.933, 0.698. The transformed (and normalized) coordinates of the rest of the oxygen atoms in the unit cell are:

0.5, 0.55, 0.715; 0.8, 0.75, 0.465; 0.7, 0.25, 0.965;
0.5, 0.45, 0.285; 0, 0.55, 0.785; 0.7, 0.75, 0.035;
0.8, 0.25, 0.535;

all also with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$. The difference in the coordinates of the two descriptions could be explained by the difference in the accuracy of the two refinements.

1.5.1.2. Change of the basis

A change of the basis is described by a (3×3) matrix:

$$\boldsymbol{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}.$$

The matrix $\boldsymbol{P}$ relates the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ to the old basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ according to

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$
$$= (\mathbf{a}P_{11} + \mathbf{b}P_{21} + \mathbf{c}P_{31},\ \mathbf{a}P_{12} + \mathbf{b}P_{22} + \mathbf{c}P_{32},\ \mathbf{a}P_{13} + \mathbf{b}P_{23} + \mathbf{c}P_{33}). \quad (1.5.1.4)$$

The matrix $\boldsymbol{P}$ is often referred to as the *linear part* of the coordinate transformation and it describes a change of direction and/or length of the basis vectors. It is preferable to choose the matrix $\boldsymbol{P}$ in such a way that its determinant is positive: a negative determinant of $\boldsymbol{P}$ implies a change from a right-handed coordinate system to a left-handed coordinate system or *vice versa*. If $\det(\boldsymbol{P}) = 0$, then the new vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ are linearly dependent, *i.e.* they do not form a complete set of basis vectors.

For a point X (*cf.* Fig. 1.5.1.1), the vector $\overrightarrow{OX} = \mathbf{x}$ is

$$\mathbf{x} = \mathbf{a}x_1 + \mathbf{b}x_2 + \mathbf{c}x_3 = \mathbf{a}'x_1' + \mathbf{b}'x_2' + \mathbf{c}'x_3' \text{ or}$$
$$\mathbf{x} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = (\mathbf{a}', \mathbf{b}', \mathbf{c}') \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}.$$

By inserting equation (1.5.1.4) one obtains

$$\mathbf{x} = (\mathbf{a}', \mathbf{b}', \mathbf{c}') \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$$

or

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix},$$

i.e. $\boldsymbol{x} = \boldsymbol{P}\boldsymbol{x}'$ or $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} = (\boldsymbol{P}, \boldsymbol{o})^{-1}\boldsymbol{x}$, which is often written as

$$\boldsymbol{x}' = \boldsymbol{Q}\boldsymbol{x} = (\boldsymbol{Q}, \boldsymbol{o})\boldsymbol{x}. \quad (1.5.1.5)$$

Here the inverse matrix $\boldsymbol{P}^{-1}$ is designated by $\boldsymbol{Q}$, while $\boldsymbol{o}$ is the (3×1) column vector with zero coefficients. [Note that in equation (1.5.1.4) the sum is over the row (first) index of $\boldsymbol{P}$, while in equation (1.5.1.5), the sum is over the column (second) index of $\boldsymbol{Q}$.]

A selected set of transformation matrices $\boldsymbol{P}$ and their inverses $\boldsymbol{P}^{-1} = \boldsymbol{Q}$ that are frequently used in crystallographic calculations are listed in Table 1.5.1.1 and illustrated in Figs. 1.5.1.2 to 1.5.1.10.

Example

Consider an *F*-centred cell with conventional basis $\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F$ and a corresponding primitive cell with basis $\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P$, *cf.* Fig. 1.5.1.4. The transformation matrix $\boldsymbol{P}$ from the conventional basis to a primitive basis can either be deduced from Fig. 1.5.1.4 or can be read directly from Table 1.5.1.1: $\mathbf{a}_P = \frac{1}{2}(\mathbf{b}_F + \mathbf{c}_F)$, $\mathbf{b}_P = \frac{1}{2}(\mathbf{a}_F + \mathbf{c}_F)$, $\mathbf{c}_P = \frac{1}{2}(\mathbf{a}_F + \mathbf{b}_F)$, which in matrix notation is

$$(\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P) = (\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F)\boldsymbol{P} = (\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F) \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}.$$

The inverse matrix $\boldsymbol{P}^{-1} = \boldsymbol{Q}$ is also listed in Table 1.5.1.1 or can be deduced from Fig. 1.5.1.4. It is the matrix that describes the conventional basis vectors $\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F$ by linear combinations of $\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P$: $\mathbf{a}_F = -\mathbf{a}_P + \mathbf{b}_P + \mathbf{c}_P$, $\mathbf{b}_F = \mathbf{a}_P - \mathbf{b}_P + \mathbf{c}_P$, $\mathbf{c}_F = \mathbf{a}_P + \mathbf{b}_P - \mathbf{c}_P$, or

$$(\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F) = (\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P)\boldsymbol{P}^{-1} = (\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P) \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

Correspondingly, the point coordinates transform as

Table 1.5.1.1
Selected 3 × 3 transformation matrices $\boldsymbol{P}$ and $\boldsymbol{Q} = \boldsymbol{P}^{-1}$

For inverse transformations (against the arrow) replace $\boldsymbol{P}$ by $\boldsymbol{Q}$ and *vice versa.*

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ C \to A \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ A \to I \end{cases}$ Unique axis **b** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to C \end{cases}$ (Fig. 1.5.1.2*a*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ B \to I \end{cases}$ Unique axis **c** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to A \end{cases}$ (Fig. 1.5.1.2*b*)	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ B \to C \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ C \to I \end{cases}$ Unique axis **a** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to B \end{cases}$ (Fig. 1.5.1.2*c*)	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **b** → unique axis **c** Cell choice 1: $\begin{cases} P \to P \\ C \to A \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **b** → unique axis **a** Cell choice 1: $\begin{cases} P \to P \\ C \to B \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ A \to C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **c** → unique axis **a** Cell choice 1: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ B \to C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
$I \to P$ (Fig. 1.5.1.3)	$\begin{pmatrix} \bar{\frac{1}{2}} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \bar{\frac{1}{2}} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	Orthorhombic Tetragonal Cubic
$F \to P$ (Fig. 1.5.1.4)	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	Orthorhombic Tetragonal Cubic

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
$(\mathbf{b}, \mathbf{a}, \bar{\mathbf{c}}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{c}, \mathbf{a}, \mathbf{b}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\bar{\mathbf{c}}, \mathbf{b}, \mathbf{a}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{b}, \mathbf{c}, \mathbf{a}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{a}, \bar{\mathbf{c}}, \mathbf{b}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$P \rightarrow C_1$, $I \rightarrow F_1$ (Fig. 1.5.1.5), **c** axis invariant	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \bar{\frac{1}{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 1.5.4.3)
$P \rightarrow C_2$, $I \rightarrow F_2$ (Fig. 1.5.1.5), **c** axis invariant	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{\frac{1}{2}} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_1, obverse setting (Fig. 1.5.1.6*a*,*c*)	$\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \bar{\frac{1}{3}} & \bar{\frac{1}{3}} \\ \frac{1}{3} & \frac{1}{3} & \bar{\frac{2}{3}} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_2, obverse setting (Fig. 1.5.1.6*c*)	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 1 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{3}} & \frac{2}{3} & \bar{\frac{1}{3}} \\ \bar{\frac{2}{3}} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_3, obverse setting (Fig. 1.5.1.6*c*)	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{3}} & \bar{\frac{1}{3}} & \frac{2}{3} \\ \frac{1}{3} & \bar{\frac{2}{3}} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_1, reverse setting (Fig. 1.5.1.6*d*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \\ 0 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{2}{3}} & \frac{1}{3} & \frac{1}{3} \\ \bar{\frac{1}{3}} & \bar{\frac{1}{3}} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_2, reverse setting (Fig. 1.5.1.6*b*,*d*)	$\begin{pmatrix} 0 & 1 & 1 \\ \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \bar{\frac{2}{3}} & \frac{1}{3} \\ \frac{2}{3} & \bar{\frac{1}{3}} & \bar{\frac{1}{3}} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_3, reverse setting (Fig. 1.5.1.6*d*)	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \bar{\frac{2}{3}} \\ \bar{\frac{1}{3}} & \frac{2}{3} & \bar{\frac{1}{3}} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ orthohexagonal centred cell C_1 (Fig. 1.5.1.7)	$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{\frac{1}{2}} & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ orthohexagonal centred cell C_2 (Fig. 1.5.1.7)	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{\frac{1}{2}} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Hexagonal cell $P \rightarrow$ orthohexagonal centred cell C_3 (Fig. 1.5.1.7)	$\begin{pmatrix} 0 & \bar{2} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{2}} & 1 & 0 \\ \bar{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_1 (Fig. 1.5.1.8)	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \bar{\frac{1}{3}} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_2 (Fig. 1.5.1.8)	$\begin{pmatrix} 2 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \\ \bar{\frac{1}{3}} & \frac{2}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_3 (Fig. 1.5.1.8)	$\begin{pmatrix} 1 & \bar{2} & 0 \\ 2 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{3}} & \frac{2}{3} & 0 \\ \bar{\frac{2}{3}} & \frac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple rhombohedral cell D_1	$\begin{pmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \bar{\frac{1}{3}} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ \bar{\frac{1}{3}} & \bar{\frac{1}{3}} & \frac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple rhombohedral cell D_2	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{2}{3}} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \bar{\frac{2}{3}} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \frac{2}{3} & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ \bar{\frac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{3}{2} & 0 & 0 \\ \bar{\frac{1}{2}} & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \bar{\frac{1}{3}} & \bar{1} & 0 \\ \frac{1}{3} & \bar{1} & 0 \\ \bar{\frac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{3}{2}} & \frac{3}{2} & 0 \\ \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 0 \\ \bar{1} & 1 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \bar{\frac{1}{3}} & 1 & 0 \\ \bar{\frac{2}{3}} & 0 & 0 \\ \bar{\frac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{\frac{3}{2}} & 0 \\ 1 & \bar{\frac{1}{2}} & 0 \\ 0 & \bar{1} & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \frac{2}{3} & 0 \\ 0 & \frac{1}{3} & 1 \\ 1 & \bar{\frac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 1 \\ \frac{3}{2} & 0 & 0 \\ \bar{\frac{1}{2}} & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \bar{\frac{1}{3}} & \bar{1} \\ 0 & \frac{1}{3} & \bar{1} \\ 1 & \bar{\frac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \bar{\frac{3}{2}} & \frac{3}{2} & 0 \\ \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \bar{\frac{1}{3}} & 1 \\ 0 & \bar{\frac{2}{3}} & 0 \\ 1 & \bar{\frac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 0 & \bar{\frac{3}{2}} & 0 \\ 1 & \bar{\frac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{\frac{1}{2}} & \bar{\frac{1}{2}} \\ 0 & \frac{1}{2} & \bar{\frac{1}{2}} \\ 1 & 0 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{2}} & 1 & \bar{\frac{1}{2}} \\ \bar{\frac{1}{2}} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Primitive rhombohedral cell → *C*-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig.1.5.1.10*b*)	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{\frac{1}{2}} & \bar{\frac{1}{2}} \\ 0 & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 1.5.1.10*b*)	$\begin{pmatrix} 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{\frac{1}{2}} & 1 & \bar{\frac{1}{2}} \\ \bar{\frac{1}{2}} & 0 & \frac{1}{2} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 1.5.1.10*b*)	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 1 \\ \frac{1}{2} & \bar{\frac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)

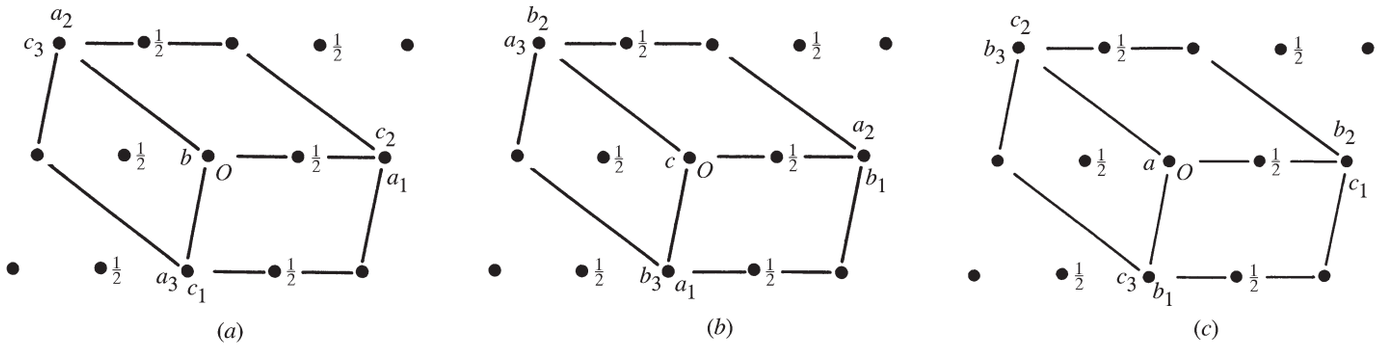


Figure 1.5.1.2
Monoclinic centred lattice, projected along the unique axis. The origin for all the cells is the same. The fractions $\frac{1}{2}$ indicate the height of the lattice points along the axis of projection.

(*a*) Unique axis *b*:
Cell choice 1: *C*-centred cell a_1, b, c_1.
Cell choice 2: *A*-centred cell a_2, b, c_2.
Cell choice 3: *I*-centred cell a_3, b, c_3.

(*b*) Unique axis *c*:
Cell choice 1: *A*-centred cell a_1, b_1, c.
Cell choice 2: *B*-centred cell a_2, b_2, c.
Cell choice 3: *I*-centred cell a_3, b_3, c.

(*c*) Unique axis *a*:
Cell choice 1: *B*-centred cell a, b_1, c_1.
Cell choice 2: *C*-centred cell a, b_2, c_2.
Cell choice 3: *I*-centred cell a, b_3, c_3.

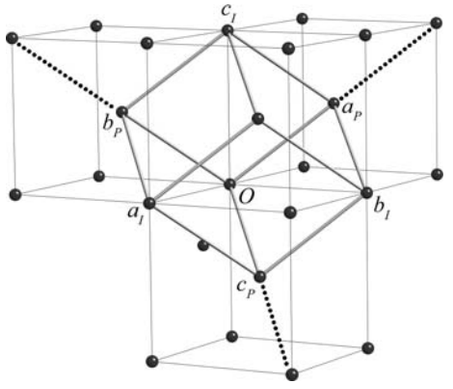


Figure 1.5.1.3
Body-centred cell *I* with a_I, b_I, c_I and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *I* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{3}$ and $\alpha = 109.47^\circ$ (rhombohedral axes) or a triple hexagonal cell with $a_{\rm hex} = a_c\sqrt{2}$ and $c_{\rm hex} = a_c \frac{1}{2}\sqrt{3}$ (hexagonal axes).

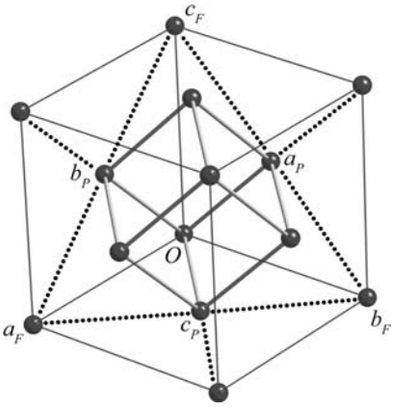


Figure 1.5.1.4
Face-centred cell *F* with a_F, b_F, c_F and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *F* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{2}$ and $\alpha = 60^\circ$ (rhombohedral axes) or a triple hexagonal cell with $a_{\rm hex} = a_c \frac{1}{2}\sqrt{2}$ and $c_{\rm hex} = a_c\sqrt{3}$ (hexagonal axes).

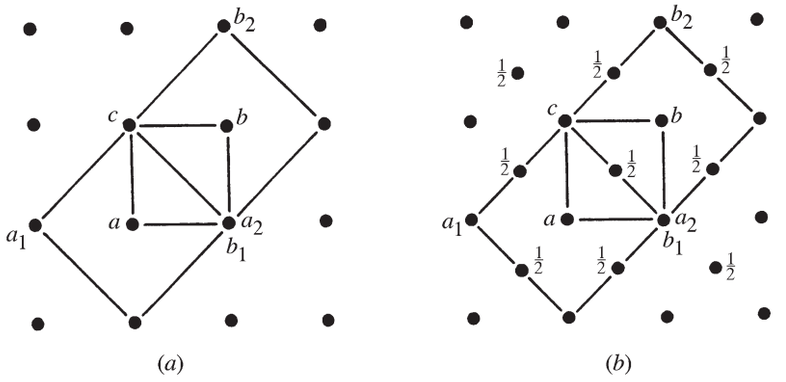


Figure 1.5.1.5
Tetragonal lattices, projected along $[00\bar{1}]$. (*a*) Primitive cell P with a, b, c and the C-centred cells C_1 with a_1, b_1, c and C_2 with a_2, b_2, c. The origin for all three cells is the same. (*b*) Body-centred cell I with a, b, c and the F-centred cells F_1 with a_1, b_1, c and F_2 with a_2, b_2, c. The origin for all three cells is the same. The fractions $\frac{1}{2}$ indicate the height of the lattice points along the axis of projection.

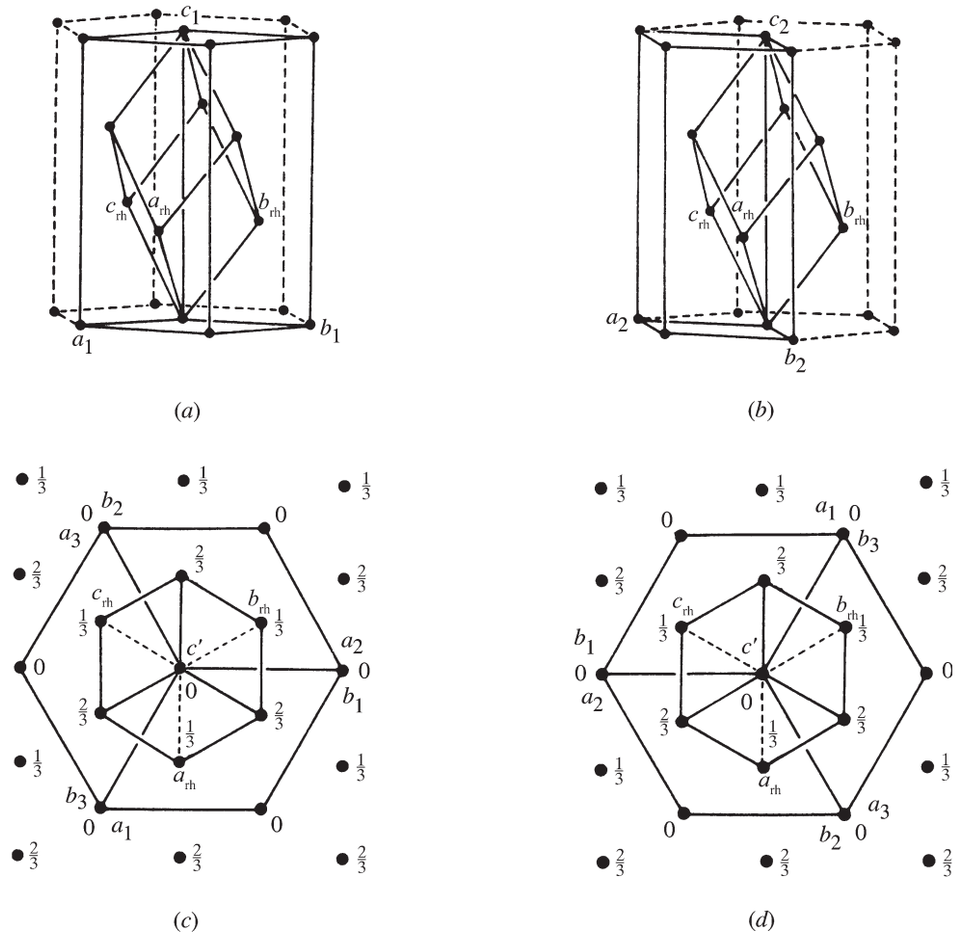


Figure 1.5.1.6
Unit cells in the rhombohedral lattice: same origin for all cells. The basis of the rhombohedral cell is labelled a_{rh}, b_{rh}, c_{rh}. Two settings of the triple hexagonal cell are possible with respect to a primitive rhombohedral cell: The *obverse setting* with the lattice points 0, 0, 0; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ has been used in *International Tables* since 1952. Its general reflection condition is $-h + k + l = 3n$. The *reverse setting* with lattice points 0, 0, 0; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$ was used in the 1935 edition. Its general reflection condition is $h - k + l = 3n$. The fractions indicate the height of the lattice points along the axis of projection. (*a*) Obverse setting of triple hexagonal cell a_1, b_1, c_1 in relation to the primitive rhombohedral cell a_{rh}, b_{rh}, c_{rh}. (*b*) Reverse setting of triple hexagonal cell a_2, b_2, c_2 in relation to the primitive rhombohedral cell a_{rh}, b_{rh}, c_{rh}. (*c*) Primitive rhombohedral cell (- - - lower edges), a_{rh}, b_{rh}, c_{rh} in relation to the three triple hexagonal cells in obverse setting a_1, b_1, c'; a_2, b_2, c'; a_3, b_3, c'. Projection along c'. (*d*) Primitive rhombohedral cell (- - - lower edges), a_{rh}, b_{rh}, c_{rh} in relation to the three triple hexagonal cells in reverse setting a_1, b_1, c'; a_2, b_2, c'; a_3, b_3, c'. Projection along c'.

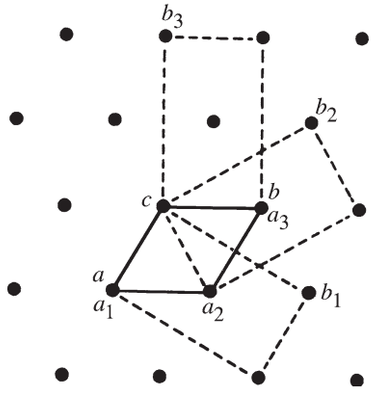


Figure 1.5.1.7
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three C-centred (orthohexagonal) cells a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.

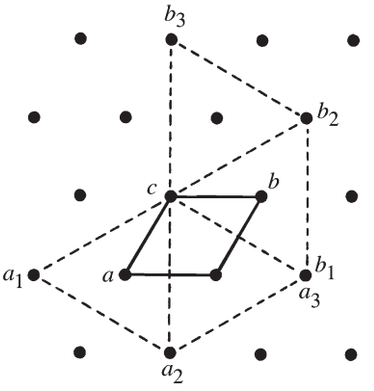
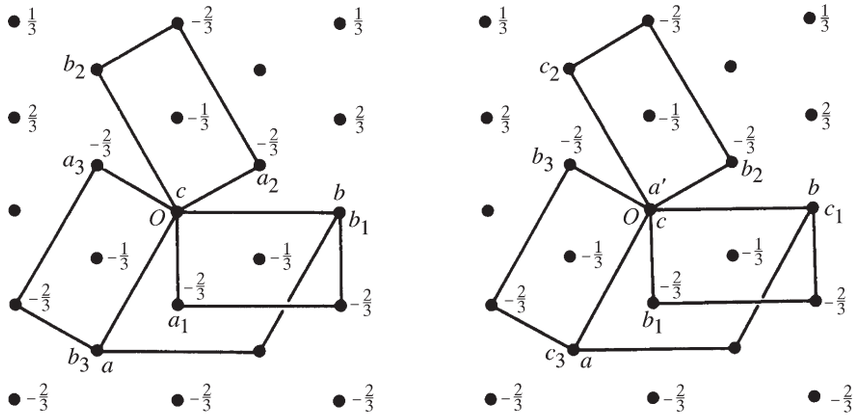
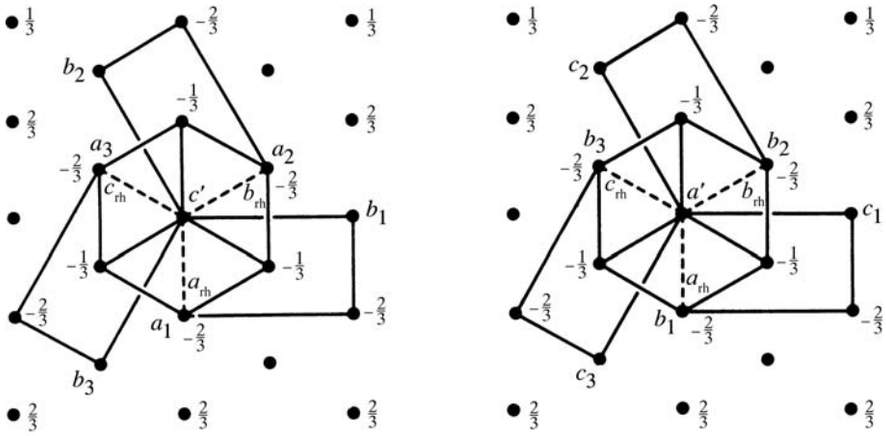


Figure 1.5.1.8
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three triple hexagonal cells H with a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.



(*a*) (*b*)

Figure 1.5.1.9
Rhombohedral lattice with a triple hexagonal unit cell a, b, c in obverse setting (*i.e.* unit cell a_1, b_1, c in Fig. 1.5.1.6*c*) and the three centred monoclinic cells. (*a*) C-centred cells C_1 with a_1, b_1, c; C_2 with a_2, b_2, c; and C_3 with a_3, b_3, c. The unique monoclinic axes are b_1, b_2 and b_3, respectively. The origin for all four cells is the same. (*b*) A-centred cells A_1 with a', b_1, c_1; A_2 with a', b_2, c_2; and A_3 with a', b_3, c_3. The unique monoclinic axes are c_1, c_2 and c_3, respectively. The origin for all four cells is the same. The fractions indicate the height of the lattice points along the axis of projection.



(*a*) (*b*)

Figure 1.5.1.10
Rhombohedral lattice with primitive rhombohedral cell a_{rh}, b_{rh}, c_{rh} and the three centred monoclinic cells. (*a*) C-centred cells C_1 with a_1, b_1, c'; C_2 with a_2, b_2, c'; and C_3 with a_3, b_3, c'. The unique monoclinic axes are b_1, b_2 and b_3, respectively. The origin for all four cells is the same. (*b*) A-centred cells A_1 with a', b_1, c_1; A_2 with a', b_2, c_2; and A_3 with a', b_3, c_3. The unique monoclinic axes are c_1, c_2 and c_3, respectively. The origin for all four cells is the same. The fractions indicate the height of the lattice points along the axis of projection.

$$\begin{pmatrix} x_P \\ y_P \\ z_P \end{pmatrix} = \boldsymbol{P}^{-1}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} -x_F + y_F + z_F \\ x_F - y_F + z_F \\ x_F + y_F - z_F \end{pmatrix}.$$

For example, the coordinates $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_F$ of the end point of $\mathbf{a}_F$ with respect to the conventional basis become $\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}_P$ in the primitive basis, the centring point $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}_F$ of the $\mathbf{a}_F, \mathbf{b}_F$ plane becomes the end point $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_P$ of $\mathbf{c}_P$ *etc.*

The concise notation of the transformation matrices is widely used in the tables of maximal subgroups of space groups in *International Tables for Crystallography* Volume A1 (2010), where $(\boldsymbol{P}, \boldsymbol{p})$ describes the relation between the conventional bases of a group and its maximal subgroups. For example, the expression $(\boldsymbol{P}, \boldsymbol{p}) = (\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}; 0, 0, \frac{1}{2})$ (*cf.* the table of maximal subgroups of $P\bar{4}2m$, No. 111, in Volume A1) stands for

$$\boldsymbol{P} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \text{ and } \boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}.$$

Note that the matrix elements of $\boldsymbol{P}$ in equation (1.5.1.8) are read by *columns* since they act on the *row* matrices of basis vectors, and not by *rows*, as in the shorthand notation of symmetry operations which apply to *column* matrices of coordinates (*cf.* Section 1.2.2.1).

1.5.1.3. General change of coordinate system

A general change of the coordinate system involves both an origin shift and a change of the basis. Such a transformation of the coordinate system is described by the matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$, where the (3×3) matrix $\boldsymbol{P}$ relates the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ to the old one $\mathbf{a}, \mathbf{b}, \mathbf{c}$ according to equation (1.5.1.4). The origin shift is described by the *shift vector* $\mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}$. The coordinates of the new origin O' with respect to the old coordinate system $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are given by the (3×1) column $\boldsymbol{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$.

The general coordinate transformation can be performed in two consecutive steps. Because the origin shift $\boldsymbol{p}$ refers to the old basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$, it has to be applied first (as described in Section 1.5.1.1), followed by the change of the basis (*cf.* Section 1.5.1.2):

$$\boldsymbol{x}' = (\boldsymbol{P}, \boldsymbol{o})^{-1}(\boldsymbol{I}, \boldsymbol{p})^{-1}\boldsymbol{x} = ((\boldsymbol{I}, \boldsymbol{p})(\boldsymbol{P}, \boldsymbol{o}))^{-1}\boldsymbol{x} = (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x}. \quad (1.5.1.6)$$

Here, $\boldsymbol{I}$ is the three-dimensional unit matrix and $\boldsymbol{o}$ is the (3×1) column matrix containing only zeros as coefficients.

The formulae for the change of the *point coordinates* from $\boldsymbol{x}$ to $\boldsymbol{x}'$ uses $(\boldsymbol{Q}, \ \boldsymbol{q}) = (\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{P}^{-1}, \ -\boldsymbol{P}^{-1}\boldsymbol{p})$, *i.e.*

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}$$

with $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ and $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$,

thus $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p})$. (1.5.1.7)

The effect of a general change of the coordinate system $(\boldsymbol{P}, \boldsymbol{p})$ on the coefficients of a vector $\mathbf{r}$ is reduced to the linear transformation described by $\boldsymbol{P}$, as the vector coefficients are not affected by the origin shift [*cf.* equation (1.5.1.3)].

Hereafter, the data for the matrix–column pair

$$(\boldsymbol{P}, \boldsymbol{p}) = \left(\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}, \ \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}\right)$$

are often written in the following concise form:

$$P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \ \ P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \ \ P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}; \ \ p_1, p_2, p_3. \quad (1.5.1.8)$$

1.5.2. Transformations of crystallographic quantities under coordinate transformations

By H. Wondratschek and M. I. Aroyo

1.5.2.1. Covariant and contravariant quantities

If the *direct* or *crystal* basis is transformed by the transformation matrix $\boldsymbol{P}$: $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$, the corresponding basis vectors of the *reciprocal (or dual) basis* transform as (*cf.* Section 1.3.2.5)

$$\begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}, \quad (1.5.2.1)$$

where the notation $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ is applied (*cf.* Section 1.5.1.2).

The quantities that transform in the same way as the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are called *covariant* with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and *contravariant* with respect to the reciprocal basis $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$. Such quantities are the *Miller indices* (hkl) of a plane (or a set of planes) in direct space and the vector coefficients (h, k, l) of the vector perpendicular to those planes, referred to the reciprocal basis $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$:

$$(h', k', l') = (h, k, l)\boldsymbol{P}. \quad (1.5.2.2)$$

Quantities like the vector coefficients of any vector $\boldsymbol{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}$ in direct space (or the *indices of a direction* in direct space) are covariant with respect to the basis vectors $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$ and contravariant with respect to $\mathbf{a}, \mathbf{b}, \mathbf{c}$:

$$\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} u \\ v \\ w \end{pmatrix}. \quad (1.5.2.3)$$

1.5.2.2. Metric tensors of direct and reciprocal lattices

The metric tensor of a crystal lattice with a basis **a**, **b**, **c** is the (3 × 3) matrix

$$\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix},$$

which can formally be described as

$$\boldsymbol{G} = (\mathbf{a},\mathbf{b},\mathbf{c})^T\cdot(\mathbf{a},\mathbf{b},\mathbf{c}) = \begin{pmatrix}\mathbf{a}\\ \mathbf{b}\\ \mathbf{c}\end{pmatrix}\cdot(\mathbf{a},\mathbf{b},\mathbf{c})$$

(*cf.* Section 1.3.2). The transformation of the metric tensor under the coordinate transformation $(\boldsymbol{P},\boldsymbol{p})$ follows directly from its definition:

$$\begin{aligned}\boldsymbol{G}' &= (\mathbf{a}',\mathbf{b}',\mathbf{c}')^T\cdot(\mathbf{a}',\mathbf{b}',\mathbf{c}') = [(\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P}]^T\cdot(\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P}\\ &= \boldsymbol{P}^T(\mathbf{a},\mathbf{b},\mathbf{c})^T\cdot(\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P} = \boldsymbol{P}^T\boldsymbol{G}\boldsymbol{P},\end{aligned} \tag{1.5.2.4}$$

where $\boldsymbol{P}^T$ is the transposed matrix of $\boldsymbol{P}$. The transformation behaviour of $\boldsymbol{G}$ under $(\boldsymbol{P},\boldsymbol{p})$ is determined by the matrix $\boldsymbol{P}$, *i.e.* $\boldsymbol{G}$ is not affected by an origin shift $\boldsymbol{p}$.

The volume V of the unit cell defined by the basis vectors **a**, **b**, **c** can be obtained from the determinant of the metric tensor, $V^2 = \det(\boldsymbol{G})$. The transformation behaviour of V under a coordinate transformation follows from the transformation behaviour of the metric tensor [note that $\det(\boldsymbol{P}) = \det(\boldsymbol{P}^T)$]: $(V')^2 = \det(\boldsymbol{G}') = \det(\boldsymbol{P}^T\boldsymbol{G}\boldsymbol{P}) = \det(\boldsymbol{P})\det(\boldsymbol{P}^T)\det(\boldsymbol{G}) = \det(\boldsymbol{P})^2V^2$, *i.e.*

$$V' = |\det(\boldsymbol{P})|V, \tag{1.5.2.5}$$

which is reduced to $V' = \det(\boldsymbol{P})V$ if $\det(\boldsymbol{P}) > 0$.

Similarly, the metric tensor $\boldsymbol{G}^*$ of the reciprocal lattice and the volume V^* of the unit cell defined by the basis vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ transform as

$$\boldsymbol{G}^{*\prime} = \boldsymbol{Q}\boldsymbol{G}^*\boldsymbol{Q}^T, \tag{1.5.2.6}$$

$$V^{*\prime} = |\det(\boldsymbol{Q})|V^* \text{ or } V^{*\prime} = \det(\boldsymbol{Q})V^* = [1/\det(\boldsymbol{P})]V^* \text{ if } \det(\boldsymbol{Q}) > 0. \tag{1.5.2.7}$$

Again, it is only the linear part $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ that determines the transformation behaviour of $\boldsymbol{G}^*$ and V^* under coordinate transformations.

1.5.2.3. Transformation of matrix–column pairs of symmetry operations

The *matrix–column pairs for the symmetry operations* are changed by a change of the coordinate system (see Section 1.2.2 for details of the matrix description of symmetry operations). A symmetry operation W that maps a point X to an image point $\tilde{X}$ is described in the 'old' (unprimed) coordinate system by the system of equations

$$\begin{aligned}\tilde{x_1} &= W_{11}x_1 + W_{12}x_2 + W_{13}x_3 + w_1\\ \tilde{x_2} &= W_{21}x_1 + W_{22}x_2 + W_{23}x_3 + w_2\\ \tilde{x_3} &= W_{31}x_1 + W_{32}x_2 + W_{33}x_3 + w_3,\end{aligned} \tag{1.5.2.8}$$

i.e. by the matrix–column pair $(\boldsymbol{W},\boldsymbol{w})$:

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} = (\boldsymbol{W},\boldsymbol{w})\boldsymbol{x}. \tag{1.5.2.9}$$

In the new (primed) coordinate system, the symmetry operation W is described by the pair $(\boldsymbol{W}',\boldsymbol{w}')$:

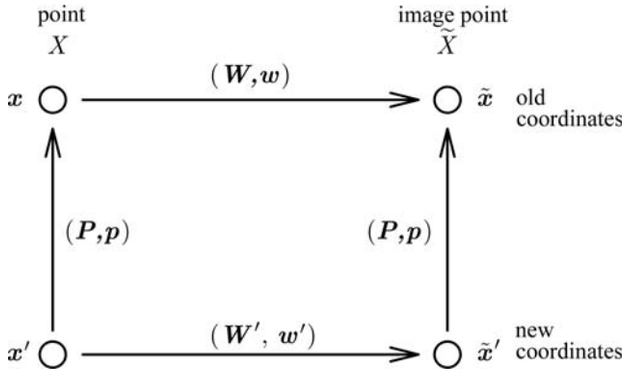


Figure 1.5.2.1
Illustration of the transformation of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$, also called a 'mapping of mappings'.

$$\tilde{\boldsymbol{x}}' = (\boldsymbol{W}',\boldsymbol{w}')\boldsymbol{x}' = \boldsymbol{W}'\boldsymbol{x}' + \boldsymbol{w}'. \tag{1.5.2.10}$$

The relation between $(\boldsymbol{W},\boldsymbol{w})$ and $(\boldsymbol{W}',\boldsymbol{w}')$ is derived *via* the transformation matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$, which specifies the change of the coordinate system. The successive application of equations (1.5.1.7), (1.5.2.9) and again (1.5.1.7) results in $\tilde{\boldsymbol{x}}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$, which compared with equation (1.5.2.10) gives

$$(\boldsymbol{W}',\boldsymbol{w}') = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}). \tag{1.5.2.11}$$

The result indicates that the change of the matrix–column pairs of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$ under a coordinate transformation described by the matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$ is realized by the conjugation of $(\boldsymbol{W},\boldsymbol{w})$ by $(\boldsymbol{P},\boldsymbol{p})$. The multiplication of the matrix–column pairs on the *right-hand side* of equation (1.5.2.11), namely $(\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1},-\boldsymbol{P}^{-1}\boldsymbol{p})(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1}\boldsymbol{W},\boldsymbol{P}^{-1}\boldsymbol{w}-\boldsymbol{P}^{-1}\boldsymbol{p})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P},\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{p}+\boldsymbol{P}^{-1}\boldsymbol{w}-\boldsymbol{P}^{-1}\boldsymbol{p})$, results in the factorization of the relation (1.5.2.11) into a pair of equations for the rotation and translation parts of $(\boldsymbol{W}',\boldsymbol{w}')$:

$$\boldsymbol{W}' = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{W}\boldsymbol{P} \tag{1.5.2.12}$$

and

$$\begin{aligned}\boldsymbol{w}' &= \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{p} + \boldsymbol{P}^{-1}\boldsymbol{w} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{w} + \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p})\\ &= \boldsymbol{Q}(\boldsymbol{w} + \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p}) = \boldsymbol{Q}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}).\end{aligned} \tag{1.5.2.13}$$

The whole formalism described above can be visualized by means of an instructive diagram, Fig. 1.5.2.1, displaying the transformation of the matrix–column pairs of symmetry operations under coordinate transformations, the so-called *mapping of mappings*.

The points X (left) and $\tilde{X}$ (right), and the corresponding columns of coordinates $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$, and $\boldsymbol{x}'$ and $\tilde{\boldsymbol{x}}'$, are referred to the old and to the new coordinate systems, respectively. The transformation matrices of each step are indicated next to the edges of the diagram, while the arrows indicate the direction, *e.g.* $\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$ but $\boldsymbol{x}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\boldsymbol{x}$. From $\boldsymbol{x}'$ to $\tilde{\boldsymbol{x}}'$ it is possible to proceed in two different ways:
(i) $\tilde{\boldsymbol{x}}' = (\boldsymbol{W}',\boldsymbol{w}')\boldsymbol{x}'$,
(ii) $\tilde{\boldsymbol{x}}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$.
The comparison of (i) and (ii) yields equation (1.5.2.11).

1.5.2.4. Augmented-matrix formalism

The augmented-matrix formalism (*cf.* Section 1.2.2) simplifies the equations of the coordinate transformations discussed above.

The matrices $\boldsymbol{P}$, $\boldsymbol{Q}$ may be combined with the corresponding columns $\boldsymbol{p}$, $\boldsymbol{q}$ to form (4×4) matrices:

$$\mathbb{P} = \left(\begin{array}{c|c} \boldsymbol{P} & \boldsymbol{p} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{Q} = \mathbb{P}^{-1} = \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \qquad (1.5.2.14)$$

where $\boldsymbol{0}$ is a 1×3 row with zero coefficients. As already indicated in Section 1.2.2, the horizontal and vertical lines in the augmented matrices have no mathematical meaning; they serve as guide to the eye so that the coefficients can be recognized more easily.

Analogously, the (3×1) columns $\boldsymbol{x}$ and $\boldsymbol{x}'$ are augmented to (4×1) columns by adding '1' as fourth coordinate in order to enable matrix multiplication with the augmented matrices: $\mathbb{x} = \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix}$; $\mathbb{x}' = \begin{pmatrix} x'_1 \\ x'_2 \\ \underline{x'_3} \\ 1 \end{pmatrix}$. Using the augmented matrices, the transformation behaviour of point coordinates [*cf.* equation (1.5.1.7)] takes the form

$$\begin{aligned} \mathbb{x}' = \mathbb{P}^{-1}\mathbb{x} = \mathbb{Q}\mathbb{x} &= \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix} \\ &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} Q_{11}x_1 + Q_{12}x_2 + Q_{13}x_3 + q_1 \\ Q_{21}x_1 + Q_{22}x_2 + Q_{23}x_3 + q_2 \\ \underline{Q_{31}x_1 + Q_{32}x_2 + Q_{33}x_3 + q_3} \\ 1 \end{pmatrix}. \end{aligned} \qquad (1.5.2.15)$$

The difference in the transformation behaviour of point coordinates and vector coefficients under coordinate transformations becomes obvious if the augmented-matrix formalism is applied. The (3×1) column of coefficients of a vector between points X and Y,

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix},$$

is augmented by adding *zero* as fourth coefficient:

$$\mathbb{r} = \mathbb{y} - \mathbb{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ \underline{y_3 - x_3} \\ 0 \end{pmatrix},$$

and this specific form of $\mathbb{r}$ reflects its specific transformation properties, namely that it is unaffected by origin shifts:

$$\begin{aligned} \mathbb{r}' = \mathbb{P}^{-1}\mathbb{r} = \mathbb{Q}\mathbb{r} &= \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) \begin{pmatrix} r_1 \\ r_2 \\ \underline{r_3} \\ 0 \end{pmatrix} \\ &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} r_1 \\ r_2 \\ \underline{r_3} \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} Q_{11}r_1 + Q_{12}r_2 + Q_{13}r_3 \\ Q_{21}r_1 + Q_{22}r_2 + Q_{23}r_3 \\ \underline{Q_{31}r_1 + Q_{32}r_2 + Q_{33}r_3} \\ 0 \end{pmatrix}. \end{aligned} \qquad (1.5.2.16)$$

The Miller indices (hkl) are coefficients of vectors in reciprocal space (plane normals). Therefore, the (1×3) rows (hkl) are augmented by 0: $(hkl|0)$. Thus, only the linear part $\boldsymbol{P}$ of the general coordinate transformation $(\boldsymbol{P}, \boldsymbol{p})$ acts on the Miller indices while the origin shift has no effect, *cf.* equation (1.5.2.2).

The augmented-matrix formulation of transformation of symmetry operations (1.5.2.11) is straightforward if the matrices $\boldsymbol{W}$ and $\boldsymbol{W}'$ are combined with the corresponding columns $\boldsymbol{w}$ and $\boldsymbol{w}'$ to form (4×4) matrices:

$$\mathbb{W} = \left(\begin{array}{c|c} \boldsymbol{W} & \boldsymbol{w} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{W}' = \left(\begin{array}{c|c} \boldsymbol{W}' & \boldsymbol{w}' \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} W'_{11} & W'_{12} & W'_{13} & w'_1 \\ W'_{21} & W'_{22} & W'_{23} & w'_2 \\ W'_{31} & W'_{32} & W'_{33} & w'_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Thus, equation (1.5.2.11) is replaced by its (4×4) analogue:

$$\begin{aligned} \mathbb{W}' = \mathbb{P}^{-1}\mathbb{W}\mathbb{P} = \mathbb{Q}\mathbb{W}\mathbb{P} &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \cdot \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \\ &\cdot \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \end{aligned} \qquad (1.5.2.17)$$

where $\mathbb{P}$ and $\mathbb{Q}$ are defined according to equation (1.5.2.14). [Note that to avoid any confusion that might result from equation (1.5.2.17) being displayed over more than one line, the matrix multiplication is explicitly indicated by centred dots between the matrices.] In analogy to equation (1.5.2.11), the change of the augmented matrices of symmetry operations $\mathbb{W}$ under coordinate transformations represented by the augmented matrices $\mathbb{P}$ is described by the conjugation of $\mathbb{W}$ with $\mathbb{P}$.

The transformation behaviour of the vector coefficients becomes apparent if the (distance) vector $\mathbf{v}$ is treated as a

translation vector and the transformation behaviour of the translation is considered. The corresponding translation is then described by $(\boldsymbol{I}, \boldsymbol{v})$, *i.e.* $\boldsymbol{W} = \boldsymbol{I}$, $\boldsymbol{w} = \boldsymbol{v}$. Equation (1.5.2.13) shows that the translation and thus the translation vector are not changed under an origin shift, $(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{I}, \boldsymbol{p})$, because $(\boldsymbol{I}, \boldsymbol{v})' = (\boldsymbol{I}, \boldsymbol{v})$ holds. For the same reason, under a general coordinate transformation the origin shift has no effect on the vector coefficients, *cf.* equation (1.5.2.16).

1.5.2.5. Example: paraelectric-to-ferroelectric phase transition of GeTe

Coordinate transformations are essential in the study of structural relationships between crystal structures. Consider as an example two phases **A** (*basic* or *parent* structure) and **B** (*derivative* structure) of the same compound. Let the space group $\mathcal{H}$ of **B** be a proper subgroup of the space group $\mathcal{G}$ of **A**, $\mathcal{H} < \mathcal{G}$. The relationship between the two structures is characterized by a global distortion that, in general, can be decomposed into a homogeneous strain describing the distortion of the lattice of **B** relative to that of **A** and an atomic displacement field representing the displacements of the atoms of **B** from their positions in **A**. In order to facilitate the comparison of the two structures, first the coordinate system of structure **A** is transformed by an appropriate transformation $(\boldsymbol{P}, \boldsymbol{p})$ to that of structure **B**. This new description of **A** will be called the *reference description* of structure **A** relative to structure **B**. Now, the metric tensors $\boldsymbol{G}_{\mathbf{A}}$ of the reference description of **A** and $\boldsymbol{G}_{\mathbf{B}}$ are of the same type and are distinguished only by the values of their parameters. The adaptation of structure **A** to structure **B** can be performed in two further steps. In the first step the parameter values of $\boldsymbol{G}_{\mathbf{A}}$ are adapted to those of $\boldsymbol{G}_{\mathbf{B}}$ by an affine transformation which determines the metric deformation (spontaneous strain) of structure **B** relative to structure **A**. The result is a hypothetical structure which still differs from structure **B** by atomic displacements. In the second step these displacements are balanced out by shifting the individual atoms to those of structure **B**. In other words, if $\mathbf{a}, \mathbf{b}, \mathbf{c}$ represents the basis of the parent phase, then its image under the transformation $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$ should be similar to the basis of the derivative phase $\mathbf{a}_{\mathcal{H}}, \mathbf{b}_{\mathcal{H}}, \mathbf{c}_{\mathcal{H}}$. The difference between $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and $\mathbf{a}_{\mathcal{H}}, \mathbf{b}_{\mathcal{H}}, \mathbf{c}_{\mathcal{H}}$ determines the metric deformation (spontaneous strain) accompanying the transition between the two phases. Similarly, the differences between the images X' of the atomic positions X of the basic structure under the transformation $(\boldsymbol{P}, \boldsymbol{p})$ and the atomic positions $X_{\mathcal{H}}$ of the derivative structure give the atomic displacements that occur during the phase transition.

As an example we will consider the structural phase transition of GeTe, which is of displacive type, *i.e.* the phase transition is accomplished through small atomic displacements. The room-temperature ferroelectric phase belongs to the rhombohedral space group *R*3*m* (160). At about 720 K a structural phase transition takes place to a high-symmetry paraelectric cubic phase of the NaCl type. The following descriptions of the two phases of GeTe are taken from the ICSD:

(*a*) Wiedemeier & Siemers (1989), ICSD No. 56037. The symmetry of the high-temperature phase is described by the space group $Fm\bar{3}m$ (225) with cell parameters a_c = 6.009 Å and atomic coordinates listed as
Ge: 4*a* 0, 0, 0
Te: 4*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

(*b*) Chattopadhyay *et al.* (1987), ICSD No. 56038. The structure is described with respect to the hexagonal-axes setting of *R*3*m* (160) (*cf.* Section 1.5.3.1) with cell parameters $a_{\rm hex}$ = 4.164 (2) Å, $c_{\rm hex}$ = 10.69 (4) Å. The coordinates of the atoms in the asymmetric unit are given as
Ge: 3*a* 0, 0, 0.2376
Te: 3*a* 0, 0, 0.7624

The relation between the basis $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ of the *F*-centred cubic lattice and the basis $\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c$ of the reference description can be obtained by inspection. The $\mathbf{c}'_c$ axis of the reference hexagonal basis must be one of the cubic threefold axes, say [111]. The axes $\mathbf{a}'_c$ and $\mathbf{b}'_c$ must be lattice vectors of the *F*-centred lattice, perpendicular to the rhombohedral axis. They must have equal length, form an angle of 120°, and together with $\mathbf{c}'_c$ define a right-handed basis. For example, the vectors $\mathbf{a}'_c = \frac{1}{2}(-\mathbf{a}_c + \mathbf{b}_c)$, $\mathbf{b}'_c = \frac{1}{2}(-\mathbf{b}_c + \mathbf{c}_c)$ fulfil these conditions.

The transformation matrix $\boldsymbol{P}$ between the bases $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ and $\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c$ can also be derived from the data listed in Table 1.5.1.1 in two steps:

(i) A cubic *F* cell can be considered as a primitive rhombohedral cell with $a_p = a_c \frac{1}{2}\sqrt{2}$ and α = 60°. The relation between the two cells is described by the transformation matrix $\boldsymbol{P}_1$ (*cf.* Table 1.5.1.1 and Fig. 1.5.1.4):

$$(\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\boldsymbol{P}_1 = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}. \tag{1.5.2.18}$$

(ii) The transformation matrix $\boldsymbol{P}_2$ between the rhombohedral primitive cell and the triple hexagonal cell (obverse setting) of the reference description is read from Table 1.5.1.1 (*cf.* Fig. 1.5.1.6):

$$(\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c) = (\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)\boldsymbol{P}_2 = (\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}. \tag{1.5.2.19}$$

Combining equations (1.5.2.18) and (1.5.2.19) gives the orientational relationship between the *F*-centred cubic cell and the rhombohedrally centred hexagonal cell $(\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\boldsymbol{P}$, where

$$\boldsymbol{P} = \boldsymbol{P}_1\boldsymbol{P}_2 = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & 0 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 1 \\ 0 & \frac{1}{2} & 1 \end{pmatrix}. \tag{1.5.2.20}$$

Formally, the lattice parameters of the reference unit cell can be extracted from the metric tensor $\boldsymbol{G}'_c$ obtained from the metric tensor $\boldsymbol{G}_c$ transformed by $\boldsymbol{P}$, *cf.* equation (1.5.2.4):

$$\begin{aligned} \boldsymbol{G}'_c &= \boldsymbol{P}^T\boldsymbol{G}_c\boldsymbol{P} \\ &= \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} \\ 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} a_c^2 & 0 & 0 \\ 0 & a_c^2 & 0 \\ 0 & 0 & a_c^2 \end{pmatrix}\begin{pmatrix} -\frac{1}{2} & 0 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 1 \\ 0 & \frac{1}{2} & 1 \end{pmatrix} \\ &= a_c^2\begin{pmatrix} \frac{1}{2} & -\frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & 0 & 3 \end{pmatrix}, \end{aligned} \tag{1.5.2.21}$$

which gives $a'_c = a_c \frac{1}{2}\sqrt{2}$ = 4.249 Å and $c'_c = a_c\sqrt{3}$ = 10.408 Å. The comparison of these values with the experimentally deter-

mined lattice parameters of the low-symmetry phase [a_{hex} = 4.164 (2) Å, c_{hex} = 10.69 (4) Å (Chattopadhyay *et al.*, 1987)] determines the lattice deformation accompanying the displacive phase transition, which basically consists of expanding the cubic unit cell along the [111] direction. (In fact, the elongation along [111] is accompanied by a contraction in the *ab* plane that leads to an overall volume reduction of about 1.3%.)

Owing to the polar character of *R*3*m*, the symmetry conditions following from the group–subgroup relation $Fm\bar{3}m > R3m$ [*cf.* equation (1.5.2.11)] are not sufficient to determine the origin shift of the transformation between the high- and the low-symmetry space groups. The origin shift of $\boldsymbol{p} = (-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4})$ in this specific case is chosen in such a way that the relative displacements of Ge and Te are equal in size but in opposite direction along [111].

The inverse transformation matrix–column pair $(\boldsymbol{Q}, \boldsymbol{q}) = (\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{P}^{-1}, -\boldsymbol{P}^{-1}\boldsymbol{p})$ is necessary for the calculation of the atomic coordinates of the reference description X'_c. Given the matrix $\boldsymbol{P}$, its inverse $\boldsymbol{P}^{-1}$ can be calculated either directly (*i.e.* applying the algebraic procedure for inversion of a matrix) or using the inverse matrices $\boldsymbol{Q}_1 = \boldsymbol{P}_1^{-1}$ and $\boldsymbol{Q}_2 = \boldsymbol{P}_2^{-1}$ listed in Table 1.5.1.1:

$$\boldsymbol{Q} = \boldsymbol{P}^{-1} = (\boldsymbol{P}_1\boldsymbol{P}_2)^{-1} = \boldsymbol{P}_2^{-1}\boldsymbol{P}_1^{-1} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix} = \begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}. \quad (1.5.2.22)$$

(Note the change in the order of multiplication of the matrices $\boldsymbol{P}_1^{-1}$ and $\boldsymbol{P}_2^{-1}$ in $\boldsymbol{Q}$.) The corresponding origin shift $\boldsymbol{q}$ is given by

$$\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p} = -\begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} -\frac{1}{4} \\ -\frac{1}{4} \\ -\frac{1}{4} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}. \quad (1.5.2.23)$$

The atomic positions of the reference description become

$$\begin{pmatrix} x'_c \\ y'_c \\ z'_c \end{pmatrix} = \begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}.$$

The coordinates of the representative Ge atom occupying position 4*a* 0, 0, 0 in $Fm\bar{3}m$ are transformed to $0, 0, \frac{1}{4}$, while those of Te are transformed from 4*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ in $Fm\bar{3}m$ to $0, 0, \frac{3}{4}$. The comparison of these values with the experimentally determined atomic coordinates of Ge 0, 0, 0.2376 and Te 0, 0, 0.7624 reveals the corresponding atomic displacements associated with the displacive phase transition. The low-symmetry phase is a result of relative atomic displacements of the Ge and Te atoms along the polar (rhombohedral) [111] direction, giving rise to non-zero polarization along the same direction, *i.e.* the phase transition is a *paraelectric-to-ferroelectric* one.

1.5.3. Transformations between different space-group descriptions

By G. Chapuis, H. Wondratschek and M. I. Aroyo

1.5.3.1. Space groups with more than one description in this volume

In the description of the space-group symbols presented in Section 1.4.1, we have already seen that in the conventional, *unique axis b* description of monoclinic space groups, the unique symmetry direction is chosen as **b**; it is normal to **c** and **a**, which form the angle β. However, it is often the case that this standard direction is not the most appropriate choice and that another choice would be more convenient. An example of this would be when following a phase transition from an orthorhombic parent phase to a monoclinic phase. Here, it would often be preferable to keep the same orientation of the axes even if the resulting monoclinic setting is not standard.

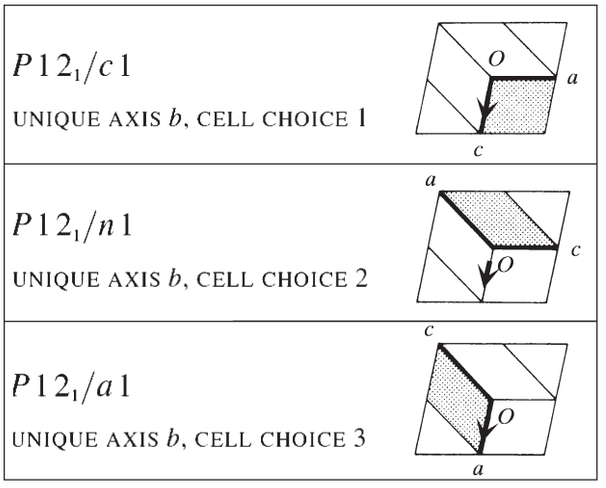


Figure 1.5.3.1
Three possible cell choices for the monoclinic space group $P2_1/c$ (14) with unique axis *b*. Note the corresponding changes in the full Hermann–Mauguin symbols. The glide vector is indicated by an arrow.

In some of the space groups, and especially in the monoclinic ones, the space-group tables of Chapter 2.3 provide a selection of possible alternative settings. For example, in space group $P2_1/c$, two possible orientations of the unit-cell axes are provided, namely with unique axis *b* and *c*. This is reflected in the corresponding full Hermann–Mauguin symbols by the explicit specification of the unique-axis position (dummy indices '1' indicate 'empty' symmetry directions), and by the corresponding change in the direction of the glide plane: $P12_1/c1$ or $P112_1/a$ (*cf.* Section 1.4.1 for a detailed treatment of Hermann–Mauguin symbols of space groups).

It is not just the unique monoclinic axis that can be varied: the choice of the other axes can vary as well. There are cases where the selection of the conventional setting leads to an inconvenient monoclinic angle that deviates greatly from 90°. If another cell choice minimizes the deviation from 90°, it is preferred. Fig. 1.5.3.1 illustrates three cell choices for the monoclinic axis *b* setting of $P2_1/c$.

In centrosymmetric space groups the origin of the unit cell is located at an inversion centre ('origin choice 2'). If, however, another point has higher site symmetry $\mathcal{S}$, a second diagram is displayed with the origin at a point with site symmetry $\mathcal{S}$ ('origin choice 1'). Fig. 1.5.3.2 illustrates the space group *Pban* with two possible origins. The origin of the first choice is located on a point with site symmetry 222, whereas the origin for the second choice is located on an inversion centre. Among the 230 space groups, this volume lists 24 centrosymmetric space groups with an additional alternative origin.

Finally, the seven rhombohedral space-group types (*i.e.* space groups with a rhombohedral lattice) also have alternative descriptions included in the space-group tables of this volume. The rhombohedral lattice is first presented with an *R*-centred

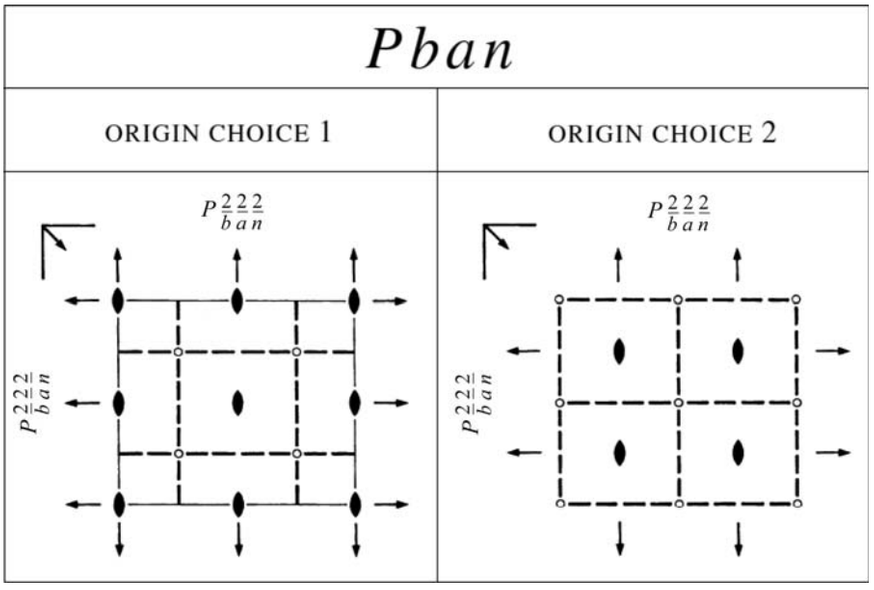


Figure 1.5.3.2
Two possible origin choices for the orthorhombic space group *Pban* (50). Origin choice 1 is on 222, whereas origin choice 2 is on $\bar{1}$.

hexagonal cell ($|\mathbf{a}_{\rm hex}| = |\mathbf{b}_{\rm hex}|$; $\mathbf{c}_{\rm hex} \perp \mathbf{a}_{\rm hex}, \mathbf{b}_{\rm hex}$; $\gamma = 120^\circ$) with a volume three times larger than that of the primitive rhombohedral cell. The second presentation is given with a primitive rhombohedral cell with $a_{\rm rh} = b_{\rm rh} = c_{\rm rh}$ and $\alpha_{\rm rh} = \beta_{\rm rh} = \gamma_{\rm rh}$. The relation between the two types of cell is illustrated in Fig. 1.5.3.3 for the space group *R*3*m* (160). In the hexagonal cell, the coordinates of the special position with site symmetry 3*m* are 0, 0, *z*, whereas in the rhombohedral cell the same special position has coordinates x, x, x. If we refer to the transformations of the primitive rhombohedral cell cited in Table 1.5.1.1, we observe two different centrings with three possible orientations R_1, R_2 and R_3 which are related by $\pm 120^\circ$ to each other. The two kinds of centrings, called *obverse* and *reverse*, are illustrated in Fig. 1.5.1.6. A rotation of 180° around the rhombohedral axis relates the obverse and reverse descriptions of the rhombohedral lattice. The obverse triple *R* cells have lattice points at $0, 0, 0$; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$, whereas the reverse *R* cells have lattice points at $0, 0, 0$; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$. The triple hexagonal cell R_1 of the obverse setting (*i.e.* $\mathbf{a}_{\rm hex} = \mathbf{a}_{\rm rh} - \mathbf{b}_{\rm rh}$, $\mathbf{b}_{\rm hex} = \mathbf{b}_{\rm rh} - \mathbf{c}_{\rm rh}$, $\mathbf{c}_{\rm hex} = \mathbf{a}_{\rm rh} + \mathbf{b}_{\rm rh} + \mathbf{b}_{\rm rh}$) has been used in the description of the rhombohedral space groups in this volume (*cf.* Table 1.5.1.1 and Fig. 1.5.3.3).

The hexagonal lattice can be referred to a centred rhombohedral cell, called the *D* cell (*cf.* Table 1.5.1.1). The centring points of this cell are $0, 0, 0$, $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ and $\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$. However, the *D* cell is rarely used in crystallography.

1.5.3.2. Examples

1.5.3.2.1. Transformations between different settings of $P2_1/c$

In the space-group tables of this volume, the monoclinic space group $P2_1/c$ (14) is described in six different settings: for each of the 'unique axis *b*' and 'unique axis *c*' settings there are three descriptions specified by different cell choices (*cf.* Section 2.1.3.15). The different settings are identified by the appropriate full Hermann–Mauguin symbols. The basis transformations $(\boldsymbol{P}, \boldsymbol{p})$ between the different settings are completely specified by the linear part of the transformation, the 3×3 matrix $\boldsymbol{P}$ [*cf.* equation (1.5.1.4)], as all settings of $P2_1/c$ refer to the same origin, *i.e.* $\boldsymbol{p} = \boldsymbol{o}$. The transformation matrices $\boldsymbol{P}$ necessary for switching between the different descriptions of $P2_1/c$ can either be read off directly or constructed from the transformation-matrix data listed in Table 1.5.1.1.

(*A*) *Transformation from $P12_1/c1$ (unique axis b, cell choice 1) to $P112_1/a$ (unique axis c, cell choice 1)*. The change of the direction of the screw axis 2_1 indicates that the unique direction **b**

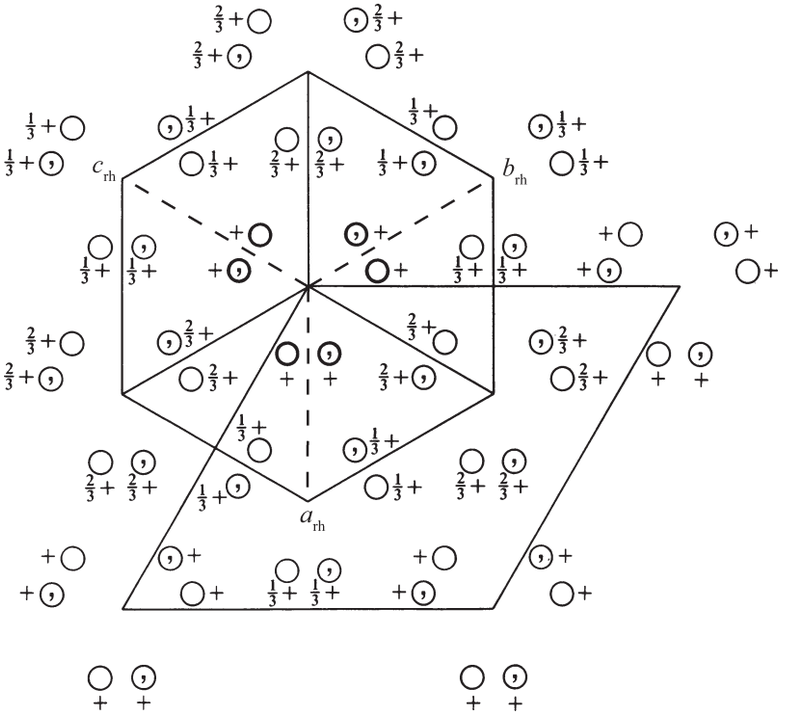


Figure 1.5.3.3
General-position diagram of the space group *R*3*m* (160) showing the relation between the hexagonal and rhombohedral axes in the obverse setting: $\mathbf{a}_{\rm rh} = \frac{1}{3}(2\mathbf{a}_{\rm hex} + \mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$, $\mathbf{b}_{\rm rh} = \frac{1}{3}(-\mathbf{a}_{\rm hex} + \mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$, $\mathbf{c}_{\rm rh} = \frac{1}{3}(-\mathbf{a}_{\rm hex} - 2\mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$.

Table 1.5.3.1
Transformation of reflection-condition data for $P12_1/c1$ to $P112_1/a$

	$P12_1/c1$ $h_bk_bl_b$	$P112_1/a$ $h_ck_cl_c$
General conditions	$h0l$: $l = 2n$ $0k0$: $k = 2n$ $00l$: $l = 2n$	$hk0$: $h = 2n$ $00l$: $l = 2n$ $h00$: $h = 2n$
Special conditions for the inversion centres	hkl: $k + l = 2n$	hkl: $h + l = 2n$

transforms to the unique direction **c**, while the glide vector along **c** transforms to a glide vector along **a**. These changes are reflected in the transformation matrix $\boldsymbol{P}$ between the basis $\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b$ of $P12_1/c1$ and $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ of $P112_1/a$, which can be read directly from Table 1.5.1.1:

$$(\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c) = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\boldsymbol{P} = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

(i) *Transformation of point coordinates*. From $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x}$, *cf.* equation (1.5.1.5), it follows that

$$\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} x_b \\ y_b \\ z_b \end{pmatrix} = \begin{pmatrix} z_b \\ x_b \\ y_b \end{pmatrix}.$$

For example, the representative coordinate triplets of the special Wyckoff position $2d\ \bar{1}$ of $P12_1/c1$ transform exactly to the representative coordinate triplets of the special Wyckoff position $2d\ \bar{1}$ of $P112_1/a$: $\begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ transform to $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$.

(ii) *Transformation of the indices in the 'Reflection conditions' block*. Under a coordinate transformation specified by a matrix $\boldsymbol{P}$, the indices of the reflection conditions (Miller indices) transform according to $(h'k'l') = (hkl)\boldsymbol{P}$, *cf.* equation (1.5.2.2). The transformation under

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

of the set of general or special reflection conditions $h_bk_bl_b$ for $P12_1/c1$ should result in the set of general or special reflection conditions $h_ck_cl_c$ of $P112_1/a$:

$$(h_ck_cl_c) = (h_bk_bl_b)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (l_bh_bk_b),$$

i.e. $h_c = l_b, k_c = h_b, l_c = k_b$ (see Table 1.5.3.1).

(iii) *Transformation of the matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$ *of the symmetry operations*. The matrices of the representatives of the symmetry operations of $P12_1/c1$ can be constructed from the coordinate triplets listed in the general-position block of the group:

(1) x, y, z (2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$

Their transformation is more conveniently performed using the augmented-matrix formalism. According to equation (1.5.2.17), the matrices $\mathbb{W}_c$ of the symmetry operations of $P112_1/a$ are related to the matrices $\mathbb{W}_b$ of $P12_1/c1$ by the equation $\mathbb{W}_c = \mathbb{Q}\mathbb{W}_b\mathbb{P}$, where

$$\mathbb{P} = \left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \quad \text{and} \quad \mathbb{Q} = \left(\begin{array}{ccc|c} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

The unit matrix representing the identity operation (1) is invariant under any basis transformation, *i.e.* x, y, z transforms to x, y, z. Similarly, the matrix of inversion $\bar{1}$ (3) (the linear part of which is a multiple of the unit matrix) is also invariant under any basis transformation, *i.e.* $\bar{x}, \bar{y}, \bar{z}$ transforms to $\bar{x}, \bar{y}, \bar{z}$. The symmetry operation (2) $\bar{x},\ y + \frac{1}{2},\ \bar{z} + \frac{1}{2}$, represented by the matrix

$$\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

transforms to

$$\left(\begin{array}{ccc|c} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)\left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$
$$= \left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

which corresponds to $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$.

Finally, the symmetry operation (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ represented by the matrix

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \text{ transforms to } \left(\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

corresponding to the coordinate triplet $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ [the matrices of (4) and its transformed are those of (2) and its transformed, multiplied by $\bar{1}$].

The coordinate triplets of the transformed symmetry operations correspond to the entries of the general-position block of $P112_1/a$ (*cf.* the space-group tables of $P2_1/c$ in Chapter 2.3).

(*B*) *Transformation from* $P112_1/b$ *(unique axis c, cell choice 3) to* $P12_1/c1$ *(unique axis b, cell choice 1)*: $(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}$. A transformation matrix from $P112_1/b$ directly to $P12_1/c1$ is not found in Table 1.5.1.1, but it can be constructed in two steps from transformation matrices that are listed there. For example:

Step 1. Unique axis *c* fixed: transformation from 'cell choice 3' to 'cell choice 1':

$$(\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1}) = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}_1 = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (1.5.3.1)$$

Step 2. Cell choice 1 invariant: transformation from unique axis c to unique axis b:

$$(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) = (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\boldsymbol{P}_2 = (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \quad (1.5.3.2)$$

The transformation matrix $\boldsymbol{P}$ for the change from $P112_1/b$ to $P12_1/c1$ is obtained by starting from equation (1.5.3.2) and replacing the expression for $\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1}$ with that from equation (1.5.3.1):

$$\begin{aligned}(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) &= (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\boldsymbol{P}_2 = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}_1\boldsymbol{P}_2 \\ &= (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\ &= (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.\end{aligned}$$

The inverse matrix $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ can be obtained either by inversion or by the product of the factors $\boldsymbol{Q}_1 = \boldsymbol{P}_1^{-1}$ and $\boldsymbol{Q}_2 = \boldsymbol{P}_2^{-1}$ but in reverse order:

$$\boldsymbol{Q} = (\boldsymbol{P}_1\boldsymbol{P}_2)^{-1} = \boldsymbol{P}_2^{-1}\boldsymbol{P}_1^{-1} = \boldsymbol{Q}_2\boldsymbol{Q}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ \bar{1} & 1 & 0 \end{pmatrix}.$$

The transformation matrix $\boldsymbol{P}$ determined above and its inverse $\boldsymbol{Q}$ permit the transformation of crystallographic data for the change from $P112_1/b$ to $P12_1/c1$.

1.5.3.2.2. Transformation between the two origin-choice settings of $I4_1/amd$

The zircon example of Section 1.5.1.1 illustrates how the atomic coordinates change under an origin-choice transformation. Here, the case of the two origin-choice descriptions of the same space group $I4_1/amd$ (141) will be used to demonstrate how the rest of the crystallographic quantities are affected by an origin shift.

The two descriptions of $I4_1/amd$ in the space-group tables of this volume are distinguished by the origin choices of the reference coordinate systems: the origin statement of the origin choice 1 setting indicates that its origin O_1 is taken at a point of $\bar{4}m2$ symmetry, which is located at $0, \frac{1}{4}, -\frac{1}{8}$ with respect to the origin O_2 of origin choice 2, taken at a centre $(2/m)$. Conversely, the origin O_2 is taken at a centre $(2/m)$ at $0, -\frac{1}{4}, \frac{1}{8}$ from the origin O_1. These origin descriptions in fact specify explicitly the origin-shift vector $\boldsymbol{p}$ necessary for the transformation between the two settings. For example, the shift vector listed for origin choice 2 expresses the origin O_2 with respect to O_1, *i.e.* the corresponding transformation matrix

$$(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{I}, \boldsymbol{p}) = \left(\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -\frac{1}{4} \\ \frac{1}{8} \end{pmatrix}\right)$$

transforms the crystallographic data from the origin choice 1 setting to the origin choice 2 setting.

(i) *Transformation of point coordinates.* In accordance with the discussion of Section 1.5.1.1 [*cf.* equation (1.5.1.2)], the transformation of point coordinates $\boldsymbol{x}_1 = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$ of the origin choice 1 setting of $I4_1/amd$ to $\boldsymbol{x}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$ of the origin choice 2 setting is given by

$$\boldsymbol{x}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} = (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x}_1 = (\boldsymbol{I}, -\boldsymbol{p})\boldsymbol{x}_1 = \begin{pmatrix} x_1 \\ y_1 + \frac{1}{4} \\ z_1 - \frac{1}{8} \end{pmatrix}. \quad (1.5.3.3)$$

(ii) *Metric tensors and the data for the reflection conditions*. The metric tensors and the data for the reflection conditions are not affected by an origin shift as $\boldsymbol{P} = \boldsymbol{I}$, *cf.* equations (1.5.2.4) and (1.5.2.2).

(iii) *Transformation of the matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$ *of the symmetry operations*. The origin-shift transformation $(\boldsymbol{I}, \boldsymbol{p})$ relates the matrix–column pairs $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ of the symmetry operations of the origin choice 1 setting of $I4_1/amd$ to $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ of the origin choice 2 setting [*cf.* equation (1.5.2.11)]:

$$(\boldsymbol{W}_2, \boldsymbol{w}_2) = (\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}_1, \boldsymbol{w}_1)(\boldsymbol{I}, \boldsymbol{p}) = (\boldsymbol{W}_1, \boldsymbol{w}_1 + [\boldsymbol{W}_1 - \boldsymbol{I}]\boldsymbol{p}). \quad (1.5.3.4)$$

The rotation part of the symmetry operation is not affected by the origin shift, but the translation part is affected, *i.e.* $\boldsymbol{W}_2 = \boldsymbol{W}_1$ and $\boldsymbol{w}_2 = \boldsymbol{w}_1 + [\boldsymbol{W}_1 - \boldsymbol{I}]\boldsymbol{p}$. For example, the translation and unit element generators of $I4_1/amd$ are not changed under the origin-shift transformation, as $\boldsymbol{W}_1 = \boldsymbol{I}$. The first non-translation generator given by the coordinate triplet $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ and represented by the matrix

$$\left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}\right) \text{ transforms to } \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} \frac{1}{4} \\ \frac{3}{4} \\ \frac{1}{4} \end{pmatrix}\right),$$

which corresponds to the coordinate triplet $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$.

The second non-translation generator $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$, represented by the matrix

$$\left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}\right) \text{ transforms to } \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\right),$$

which under the normalization $0 \leq w_i < 1$ is written as the coordinate triplet $\bar{x}, \bar{y}, \bar{z}$. The coordinate triplets of the transformed symmetry operations are the entries of the corresponding generators of the origin choice 2 setting of $I4_1/amd$ (*cf.* the space-group tables of $I4_1/amd$ in Chapter 2.3).

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

By B. Souvignier, G. Chapuis and H. Wondratschek

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 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 $W = (\boldsymbol{W}, \boldsymbol{w})$ 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 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 $\mathcal{T}W$ 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 $\boldsymbol{W}$ 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 $\boldsymbol{w}$ 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 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 $\boldsymbol{w}' = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ u_3 \end{pmatrix}$. 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 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 $\boldsymbol{w}'_g = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$ 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 W' is a coaxial equivalent of the symmetry operation $W'' = \bar{y} + u_1, x + u_2, z$, which has intrinsic translation part $\boldsymbol{o}$. To locate the geometric element of 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 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

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	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, 0$	*P*422 (89) *R*32 (155) *P*432 (207)
m	x, x, z	1, 0, 0 0, 1, 0	*g*	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, z$	*p*4*mm* (11) *P*4*mm* (99) *R*3*m* (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) *R*3*c* (161) $P\bar{4}3n$ (218)
Hexagonal coordinate system						
2	$x, 0, 0$	1, 1, 0 0, 1, 0	2_1	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, 0$	*P*321 (150) *R*32 (155)
2	$x, 2x, 0$	0, 1, 0 1, 1, 0	2_1	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, 0$	*P*312 (149) *P*622 (177)
m	$x, 2x, z$	0, 1, 0 1, 1, 0	*b*	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, z$	*P*3*m*1 (156) *p*3*m*1 (14) *R*3*m* (160)
c	$x, 2x, z$	0, 1, 0 1, 1, 0	*n*	$\frac{1}{2}, 1, \frac{1}{2}$	$x, 2x+\frac{1}{2}, z$	*P*3*c*1 (158) $P\bar{6}c2$ (188) *R*3*c* (161)
m	$x, 0, z$	1, 1, 0 0, 1, 0	*a*	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, z$	*P*31*m* (157) *p*31*m* (15)
c	$x, 0, z$	1, 1, 0 0, 1, 0	*n*	$\frac{1}{2}, 0, \frac{1}{2}$ $-\frac{1}{2}, 0, \frac{1}{2}$	$x, \frac{1}{2}, z$	*P*31*c* (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	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	$x, x+\frac{2}{3}, x+\frac{1}{3}$	*R*3 (146) *P*23 (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 *Fmm*2 (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.

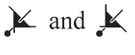
On the other hand, for an integer $u \neq 0$, the symmetry operation $W'' = z+u, x+u, y+u$ itself is a screw rotation, but it belongs to a symmetry element of rotation type, since it is a coaxial equivalent of the threefold rotation W. The crucial difference between the symmetry operations $W' = z+1, x, y$ 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}$3*m* (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}$3*c* (219)
$d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$								$d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$			*I*$\bar{4}$3*d* (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	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$	*F*4$_1$32 (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



(*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 $x+\frac{1}{2}, x, \frac{1}{4}$.

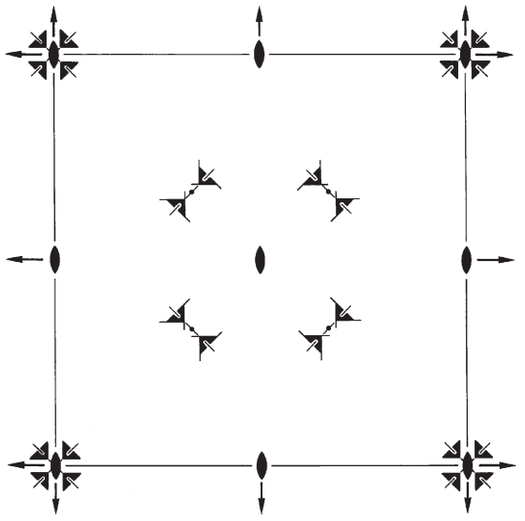


Figure 1.5.4.1
Symmetry-element diagram for space group $P23$ (195).

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 **ab**$\underline{\mathbf{c}}$ and **cb**$\underline{\bar{\mathbf{a}}}$, **ab**$\underline{\bar{\mathbf{c}}}$ and **ba**$\underline{\mathbf{c}}$, $\underline{\mathbf{a}}$**bc** and $\underline{\bar{\mathbf{a}}}$**cb**. 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.

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 *p*	1 2	1 2		*p*1 *p*2			
Rectangular *p*, *c*	*m*	3 4 5	*pm* *pg* *cm*	*p*1*m*1 *p*1*g*1 *c*1*m*1	 *c*1*m*1 *g*	*p*11*m* *p*11*g* *c*11*m*	
	2*mm*	6 7 8 9		*p*2*mm* *p*2*mg* *p*2*gg* *c*2*mm*	 *c*2*mm* *g g*	*p*2*mm* *p*2*gm* *p*2*gg* *c*2*mm*	
Square *p*	4 4*mm*	10 11 12		*p*4 *p*4*mm* *p*4*gm*	 *p*4*mm* *g* *p*4*gm* *g*		*c*4 *c*4*mm* *g* *c*4*mg* *g*
Hexagonal *p*	3 3*m*	13 14 15		*p*3 *p*3*m*1 *p*31*m*	 *p*3*m*1 *g* *p*31*m* *g*		*h*3 *h*31*m* *g* *h*3*m*1 *g*
	6 6*mm*	16 17		*p*6 *p*6*mm*	 *p*6*mm* *g g*		*h*6 *h*6*mm* *g g*

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$\bar{\mathbf{c}}$**, **cab**, **$\bar{\mathbf{c}}$ba**, **bca** and **ac$\bar{\mathbf{b}}$**. 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 *Pmm*2 (25) the permutation yields the new setting *P*2*mm*, 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 *Cmm*2 (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 *A*2*mm* setting of *Cmm*2.

The extended Hermann–Mauguin symbol of the centred space group *Aem*2 (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 *B*2*em*. Note that in the cases of the five orthorhombic space groups whose Hermann–Mauguin symbols contain the *e*-glide symbol, namely *Aem*2 (39), *Aea*2 (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 $C2/m\,2/m\,2/e$ (67) and the corresponding short symbol *Cmme*. As another example, consider the space group $C2/m\,2/c\,2_1/m$ (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 centrings, 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* centrings and by a factor of two for *I* centrings when compared to those of a space group with a

(*continued on page* 106)

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						
			abc	**cb̄a**	**abc̲**	**bac̄**	**a̲bc**	**ā̲cb**	Unique axis b Unique axis c Unique axis a
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121_1$	$A121_1$	$A112_1$	$B112_1$	$B211_1$	$C211_1$	Cell choice 1
			$A121_1$	$C121_1$	$B112_1$	$A112_1$	$C211_1$	$B211_1$	Cell choice 2
			$I121_1$	$I121_1$	$I112_1$	$I112_1$	$I211_1$	$I211_1$	Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$	$P1a1$	$P11a$	$P11b$	$Pb11$	$Pc11$	Cell choice 1
			$P1n1$	$P1n1$	$P11n$	$P11n$	$Pn11$	$Pn11$	Cell choice 2
			$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3
8	C_s^3	Cm	$C1m1$	$A1m1$	$A11m$	$B11m$	$Bm11$	$Cm11$	Cell choice 1
			$A1m1$	$C1m1$	$B11m$	$A11m$	$Cm11$	$Bm11$	Cell choice 2
			$I1m1$	$I1m1$	$I11m$	$I11m$	$Im11$	$Im11$	Cell choice 3
9	C_s^4	Cc	$C1c1$	$A1a1$	$A11a$	$B11b$	$Bb11$	$Cc11$	Cell choice 1
			$A1n1$	$C1n1$	$B11n$	$A11n$	$Cn11$	$Bn11$	Cell choice 2
			$I1a1$	$I1c1$	$I11b$	$I11a$	$Ic11$	$Ib11$	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

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						
			a$\underline{\mathbf{b}}$**c**	**c**$\bar{\mathbf{b}}$**a**	**ab**$\underline{\mathbf{c}}$	**ba**$\bar{\underline{\mathbf{c}}}$	$\underline{\mathbf{a}}$**bc**	$\bar{\underline{\mathbf{a}}}$**cb**	Unique axis *b* Unique axis *c* Unique axis *a*
14	C_{2h}^5	$P2_1/c$	$P1\frac{2_1}{c}1$	$P1\frac{2_1}{a}1$	$P11\frac{2_1}{a}$	$P11\frac{2_1}{b}$	$P\frac{2_1}{b}11$	$P\frac{2_1}{c}11$	Cell choice 1
			$P1\frac{2_1}{n}1$	$P1\frac{2_1}{n}1$	$P11\frac{2_1}{n}$	$P11\frac{2_1}{n}$	$P\frac{2_1}{n}11$	$P\frac{2_1}{n}11$	Cell choice 2
			$P1\frac{2_1}{a}1$	$P1\frac{2_1}{c}1$	$P11\frac{2_1}{b}$	$P11\frac{2_1}{a}$	$P\frac{2_1}{c}11$	$P\frac{2_1}{b}11$	Cell choice 3
15	C_{2h}^6	$C2/c$	$C1\frac{2}{c}1$	$A1\frac{2}{a}1$	$A11\frac{2}{a}$	$B11\frac{2}{b}$	$B\frac{2}{b}11$	$C\frac{2}{c}11$	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
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$	

ORTHORHOMBIC SYSTEM

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**bac̄**	**cab**	**c̄ba**	**bca**	**ac̄b**
16	D_2^1	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$
17	D_2^2	$P222_1$	$P222_1$	$P222_1$	$P2_122$	$P2_122$	$P22_12$	$P22_12$
18	D_2^3	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P22_12_1$	$P22_12_1$	$P2_122_1$	$P2_122_1$
19	D_2^4	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
20	D_2^5	$C222_1$	$C222_1$ $2_12_12_1$	$C222_1$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$B22_12$ $2_12_12_1$	$B22_12$ $2_12_12_1$
21	D_2^6	$C222$	$C222$ 2_12_12	$C222$ 2_12_12	$A222$ 22_12_1	$A222$ 22_12_1	$B222$ 2_122_1	$B222$ 2_122_1
22	D_2^7	$F222$	$F222$ 2_12_12 22_12_1 2_122_1	$F222$ 2_12_12 2_122_1 22_12_1	$F222$ 22_12_1 2_122_1 2_12_12	$F222$ 22_12_1 2_12_12 2_122_1	$F222$ 2_122_1 2_12_12 22_12_1	$F222$ 2_122_1 22_12_1 2_12_12
23	D_2^8	$I222$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$
24	D_2^9	$I2_12_12_1$	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222
25	C_{2v}^1	$Pmm2$	$Pmm2$	$Pmm2$	$P2mm$	$P2mm$	$Pm2m$	$Pm2m$
26	C_{2v}^2	$Pmc2_1$	$Pmc2_1$	$Pcm2_1$	$P2_1ma$	$P2_1am$	$Pb2_1m$	$Pm2_1b$
27	C_{2v}^3	$Pcc2$	$Pcc2$	$Pcc2$	$P2aa$	$P2aa$	$Pb2b$	$Pb2b$
28	C_{2v}^4	$Pma2$	$Pma2$	$Pbm2$	$P2mb$	$P2cm$	$Pc2m$	$Pm2a$
29	C_{2v}^5	$Pca2_1$	$Pca2_1$	$Pbc2_1$	$P2_1ab$	$P2_1ca$	$Pc2_1b$	$Pb2_1a$
30	C_{2v}^6	$Pnc2$	$Pnc2$	$Pcn2$	$P2na$	$P2an$	$Pb2n$	$Pn2b$
31	C_{2v}^7	$Pmn2_1$	$Pmn2_1$	$Pnm2_1$	$P2_1mn$	$P2_1nm$	$Pn2_1m$	$Pm2_1n$
32	C_{2v}^8	$Pba2$	$Pba2$	$Pba2$	$P2cb$	$P2cb$	$Pc2a$	$Pc2a$
33	C_{2v}^9	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$
34	C_{2v}^{10}	$Pnn2$	$Pnn2$	$Pnn2$	$P2nn$	$P2nn$	$Pn2n$	$Pn2n$
35	C_{2v}^{11}	$Cmm2$	$Cmm2$ $ba2$	$Cmm2$ $ba2$	$A2mm$ $2cb$	$A2mm$ $2cb$	$Bm2m$ $c2a$	$Bm2m$ $c2a$

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)	**bac̄**	**cab**	**c̄ba**	**bca**	**ac̄b**
36	C_{2v}^{12}	$Cmc2_1$	$Cmc2_1$ $bn2_1$	$Ccm2_1$ $na2_1$	$A2_1ma$ 2_1cn	$A2_1am$ 2_1nb	$Bb2_1m$ $n2_1a$	$Bm2_1b$ $c2_1n$
37	C_{2v}^{13}	$Ccc2$	$Ccc2$ $nn2$	$Ccc2$ $nn2$	$A2aa$ $2nn$	$A2aa$ $2nn$	$Bb2b$ $n2n$	$Bb2b$ $n2n$
38	C_{2v}^{14}	$Amm2$	$Amm2$ $nc2_1$	$Bmm2$ $cn2_1$	$B2mm$ 2_1na	$C2mm$ 2_1an	$Cm2m$ $b2_1n$	$Am2m$ $n2_1b$
39†	C_{2v}^{15}	$Aem2$	$Abm2$ ($Aem2$) $cc2_1$	$Bma2$ ($Bme2$) $cc2_1$	$B2cm$ ($B2em$) 2_1aa	$C2mb$ ($C2me$) 2_1aa	$Cm2a$ ($Cm2e$) $b2_1b$	$Ac2m$ ($Ae2m$) $b2_1b$
40	C_{2v}^{16}	$Ama2$	$Ama2$ $nn2_1$	$Bbm2$ $nn2_1$	$B2mb$ 2_1nn	$C2cm$ 2_1nn	$Cc2m$ $n2_1n$	$Am2a$ $n2_1n$
41†	C_{2v}^{17}	$Aea2$	$Aba2$ ($Aea2$) $cn2_1$	$Bba2$ ($Bbe2$) $nc2_1$	$B2cb$ ($B2eb$) 2_1an	$C2cb$ ($C2ce$) 2_1na	$Cc2a$ ($Cc2e$) $n2_1b$	$Ac2a$ ($Ae2a$) $b2_1n$
42	C_{2v}^{18}	$Fmm2$	$Fmm2$ $ba2$ $nc2_1$ $cn2_1$	$Fmm2$ $ba2$ $cn2_1$ $nc2_1$	$F2mm$ $2cb$ 2_1na 2_1an	$F2mm$ $2cb$ 2_1an 2_1na	$Fm2m$ $c2a$ $b2_1n$ $n2_1b$	$Fm2m$ $c2a$ $n2_1b$ $b2_1n$
43	C_{2v}^{19}	$Fdd2$	$Fdd2$ $dd2_1$	$Fdd2$ $dd2_1$	$F2dd$ 2_1dd	$F2dd$ 2_1dd	$Fd2d$ $d2_1d$	$Fd2d$ $d2_1d$
44	C_{2v}^{20}	$Imm2$	$Imm2$ $nn2_1$	$Imm2$ $nn2_1$	$I2mm$ 2_1nn	$I2mm$ 2_1nn	$Im2m$ $n2_1n$	$Im2m$ $n2_1n$
45	C_{2v}^{21}	$Iba2$	$Iba2$ $cc2_1$	$Iba2$ $cc2_1$	$I2cb$ 2_1aa	$I2cb$ 2_1aa	$Ic2a$ $b2_1b$	$Ic2a$ $b2_1b$
46	C_{2v}^{22}	$Ima2$	$Ima2$ $nc2_1$	$Ibm2$ $cn2_1$	$I2mb$ 2_1na	$I2cm$ 2_1an	$Ic2m$ $b2_1n$	$Im2a$ $n2_1b$
47	D_{2h}^{1}	$P\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$
48	D_{2h}^{2}	$P\frac{2}{n}\frac{2}{n}\frac{2}{n}$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$
49	D_{2h}^{3}	$P\frac{2}{c}\frac{2}{c}\frac{2}{m}$	$Pccm$	$Pccm$	$Pmaa$	$Pmaa$	$Pbmb$	$Pbmb$
50	D_{2h}^{4}	$P\frac{2}{b}\frac{2}{a}\frac{2}{n}$	$Pban$	$Pban$	$Pncb$	$Pncb$	$Pcna$	$Pcna$
51	D_{2h}^{5}	$P\frac{2_1}{m}\frac{2}{m}\frac{2}{a}$	$Pmma$	$Pmmb$	$Pbmm$	$Pcmm$	$Pmcm$	$Pmam$
52	D_{2h}^{6}	$P\frac{2}{n}\frac{2_1}{n}\frac{2}{a}$	$Pnna$	$Pnnb$	$Pbnn$	$Pcnn$	$Pncn$	$Pnan$
53	D_{2h}^{7}	$P\frac{2}{m}\frac{2}{n}\frac{2_1}{a}$	$Pmna$	$Pnmb$	$Pbmn$	$Pcnm$	$Pncm$	$Pman$
54	D_{2h}^{8}	$P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$	$Pcca$	$Pccb$	$Pbaa$	$Pcaa$	$Pbcb$	$Pbab$
55	D_{2h}^{9}	$P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$	$Pbam$	$Pbam$	$Pmcb$	$Pmcb$	$Pcma$	$Pcma$
56	D_{2h}^{10}	$P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$	$Pccn$	$Pccn$	$Pnaa$	$Pnaa$	$Pbnb$	$Pbnb$
57	D_{2h}^{11}	$P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}$	$Pbcm$	$Pcam$	$Pmca$	$Pmab$	$Pbma$	$Pcmb$
58	D_{2h}^{12}	$P\frac{2_1}{n}\frac{2_1}{n}\frac{2}{m}$	$Pnnm$	$Pnnm$	$Pmnn$	$Pmnn$	$Pnmn$	$Pnmn$
59	D_{2h}^{13}	$P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}$	$Pmmn$	$Pmmn$	$Pnmm$	$Pnmm$	$Pmnm$	$Pmnm$
60	D_{2h}^{14}	$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$	$Pbcn$	$Pcan$	$Pnca$	$Pnab$	$Pbna$	$Pcnb$
61	D_{2h}^{15}	$P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	$Pbca$	$Pcab$	$Pbca$	$Pcab$	$Pbca$	$Pcab$
62	D_{2h}^{16}	$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	$Pnma$	$Pmnb$	$Pbnm$	$Pcmn$	$Pmcn$	$Pnam$
63	D_{2h}^{17}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{m}$	$Cmcm$ bnn	$Ccmm$ nan	$Amma$ ncn	$Amam$ nnb	$Bbmm$ nna	$Bmmb$ cnn
64†	D_{2h}^{18}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{e}$	$Cmca$ ($Cmce$) bnb	$Ccmb$ ($Ccme$) naa	$Abma$ ($Aema$) ccn	$Acam$ ($Aeam$) bnb	$Bbcm$ ($Bbem$) naa	$Bmab$ ($Bmeb$) cnn

Table 1.5.4.4 (continued)

No. of space group	Schoen-flies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**bac̄**	**cab**	**c̄ba**	**bca**	**ac̄b**
65	D_{2h}^{19}	$C\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Cmmm* *ban*	*Cmmm* *ban*	*Ammm* *ncb*	*Ammm* *ncb*	*Bmmm* *cna*	*Bmmm* *cna*
66	D_{2h}^{20}	$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Cccm* *nnn*	*Cccm* *nnn*	*Amaa* *nnn*	*Amaa* *nnn*	*Bbmb* *nnn*	*Bbmb* *nnn*
67†	D_{2h}^{21}	$C\frac{2}{m}\frac{2}{m}\frac{2}{e}$	*Cmma* (*Cmme*) *bab*	*Cmmb* (*Cmme*) *baa*	*Abmm* (*Aemm*) *ccb*	*Acmm* (*Aemm*) *bcb*	*Bmcm* (*Bmem*) *caa*	*Bmam* (*Bmem*) *cca*
68†	D_{2h}^{22}	$C\frac{2}{c}\frac{2}{c}\frac{2}{e}$	*Ccca* (*Ccce*) *nnb*	*Cccb* (*Ccce*) *nna*	*Abaa* (*Aeaa*) *cnn*	*Acaa* (*Aeaa*) *bnn*	*Bbcb* (*Bbeb*) *nan*	*Bbab* (*Bbeb*) *ncn*
69	D_{2h}^{23}	$F\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Fmmm* *ban* *ncb* *cna*	*Fmmm* *ban* *cna* *ncb*	*Fmmm* *ncb* *cna* *ban*	*Fmmm* *ncb* *ban* *cna*	*Fmmm* *cna* *ban* *ncb*	*Fmmm* *cna* *ncb* *ban*
70	D_{2h}^{24}	$F\frac{2}{d}\frac{2}{d}\frac{2}{d}$	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*
71	D_{2h}^{25}	$I\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*
72	D_{2h}^{26}	$I\frac{2}{b}\frac{2}{a}\frac{2}{m}$	*I bam* *ccn*	*I bam* *ccn*	*I mcb* *naa*	*I mcb* *naa*	*I cma* *bnb*	*I cma* *bnb*
73	D_{2h}^{27}	$I\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*
74	D_{2h}^{28}	$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}$	*I mma* *nnb*	*I mmb* *nna*	*I bmm* *cnn*	*I cmm* *bnn*	*I mcm* *nan*	*I mam* *ncn*

† For the five space groups *Aem*2 (39), *Aea*2 (41), *Cmce* (64), *Cmme* (67) and *Ccce* (68), the 'new' space-group symbols, containing the symbol '*e*' for the 'double' glide plane, are given for all settings. These symbols were first introduced in the fourth edition of this volume (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 *P* or *I*		Multiple cell *C* or *F*	
		Short	Extended	Short	Extended
75	C_4^1	*P*4		*C*4	
76	C_4^2	$P4_1$		$C4_1$	
77	C_4^3	$P4_2$		$C4_2$	
78	C_4^4	$P4_3$		$C4_3$	
79	C_4^5	*I* 4	*I*4 4_2	*F*4	*F*4 4_2
80	C_4^6	$I\,4_1$	$I4_1$ 4_3	$F4_1$	$F4_1$ 4_3
81	S_4^1	$P\bar{4}$		$C\bar{4}$	
82	S_4^2	$I\bar{4}$		$F\bar{4}$	
83	C_{4h}^1	*P*4/*m*		*C*4/*m*	$C4_2/m$ *n*
84	C_{4h}^2	$P4_2/m$		$C4_2/m$	$C4_2/m$ *n*
85	C_{4h}^3	*P*4/*n*		*C*4/*e*	*C*4/*a* *b*
86	C_{4h}^4	$P4_2/n$		$C4_2/e$	$C4_2/a$ *b*
87	C_{4h}^5	*I* 4/*m*	*I*4/*m* $4_2/n$	*F*4/*m*	*F*4/*m* $4_2/a$
88	C_{4h}^6	$I\,4_1/a$	$I4_1/a$ $4_3/b$	$F4_1/d$	$F4_1/d$ $4_3/d$
89	D_4^1	*P*422	*P*422 2_1	*C*422	*C*422 2_1
90	D_4^2	$P42_12$	$P42_12$ 2_1	$C422_1$	$C422_1$ 2_1

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
91	D_4^3	$P4_122$	$P4_122$ 2_1	$C4_122$	$C4_122$ 2_1
92	D_4^4	$P4_12_12$	$P4_12_12$ 2_1	$C4_122_1$	$C4_122_1$ 2_1
93	D_4^5	$P4_222$	$P4_222$ 2_1	$C4_222$	$C4_222$ 2_1
94	D_4^6	$P4_22_12$	$P4_22_12$ 2_1	$C4_222_1$	$C4_222_1$ 2_1
95	D_4^7	$P4_322$	$P4_322$ 2_1	$C4_322$	$C4_322$ 2_1
96	D_4^8	$P4_32_12$	$P4_32_12$ 2_1	$C4_322_1$	$C4_322_1$ 2_1
97	D_4^9	$I422$	$I422$ $4_22_12_1$	$F422$	$F422$ $4_22_12_1$
98	D_4^{10}	$I4_122$	$I4_122$ $4_32_12_1$	$F4_122$	$F4_122$ $4_32_12_1$
99	C_{4v}^1	$P4mm$	$P4mm$ g	$C4mm$	$C4mm$ b
100	C_{4v}^2	$P4bm$	$P4bm$ g	$C4mg_1$	$C4mg_1$ b
101	C_{4v}^3	$P4_2cm$	$P4_2cm$ g	$C4_2mc$	$C4_2mc$ b
102	C_{4v}^4	$P4_2nm$	$P4_2nm$ g	$C4_2mg_2$	$C4_2mg_2$ b
103	C_{4v}^5	$P4cc$	$P4cc$ n	$C4cc$	$C4cc$ n
104	C_{4v}^6	$P4nc$	$P4nc$ n	$C4cg_2$	$C4cg_2$ n
105	C_{4v}^7	$P4_2mc$	$P4_2mc$ n	$C4_2cm$	$C4_2cm$ n
106	C_{4v}^8	$P4_2bc$	$P4_2bc$ n	$C4_2cg_1$	$C4_2cg_1$ n
107	C_{4v}^9	$I4mm$	$I4mm$ 4_2nc	$F4mm$	$F4mm$ 4_2cg_2
108	C_{4v}^{10}	$I4cm$	$I4cc$ 4_2bm	$F4mc$	$F4cc$ 4_2mg_1
109	C_{4v}^{11}	$I4_1md$	$I4_1md$ 4_1nd	$F4_1dm$	$F4_1dm$ 4_3dg_2
110	C_{4v}^{12}	$I4_1cd$	$I4_1cd$ 4_3bd	$F4_1dc$	$F4_1dc$ 4_3dg_1
111	D_{2d}^1	$P\bar{4}2m$	$P\bar{4}2m$ g	$C\bar{4}m2$	$C\bar{4}m2$ b
112	D_{2d}^2	$P\bar{4}2c$	$P\bar{4}2c$ n	$C\bar{4}c2$	$C\bar{4}c2$ n
113	D_{2d}^3	$P\bar{4}2_1m$	$P\bar{4}2_1m$ g	$C\bar{4}m2_1$	$C\bar{4}m2_1$ b
114	D_{2d}^4	$P\bar{4}2_1c$	$P\bar{4}2_1c$ n	$C\bar{4}c2_1$	$C\bar{4}c2_1$ n
115	D_{2d}^5	$P\bar{4}m2$	$P\bar{4}m2$ 2_1	$C\bar{4}2m$	$C\bar{4}2m$ 2_1
116	D_{2d}^6	$P\bar{4}c2$	$P\bar{4}c2$ 2_1	$C\bar{4}2c$	$C\bar{4}2c$ 2_1
117	D_{2d}^7	$P\bar{4}b2$	$P\bar{4}b2$ 2_1	$C\bar{4}2g_1$	$C\bar{4}2g_1$ 2_1
118	D_{2d}^8	$P\bar{4}n2$	$P\bar{4}n2$ 2_1	$C\bar{4}2g_2$	$C\bar{4}2g_2$ 2_1
119	D_{2d}^9	$I\bar{4}m2$	$I\bar{4}m2$ $n2_1$	$F\bar{4}2m$	$F\bar{4}2m$ 2_1g_2
120	D_{2d}^{10}	$I\bar{4}c2$	$I\bar{4}c2$ $b2_1$	$F\bar{4}2c$	$F\bar{4}2c$ 2_1n
121	D_{2d}^{11}	$I\bar{4}2m$	$I\bar{4}2m$ 2_1c	$F\bar{4}m2$	$F\bar{4}m2$ $c2_1$
122	D_{2d}^{12}	$I\bar{4}2d$	$I\bar{4}2d$ 2_1d	$F\bar{4}d2$	$F\bar{4}d2$ $d2_1$

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
123	D_{4h}^1	$P4/mmm$	$P4/m\ 2/m\ 2/m$	$C4/mmm$	$C4/mmm$
			$2_1/g$		nb
124	D_{4h}^2	$P4/mcc$	$P4/m\ 2/c\ 2/c$	$C4/mcc$	$C4/mcc$
			$2_1/n$		nn
125	D_{4h}^3	$P4/nbm$	$P4/n\ 2/b\ 2/m$	$C4/emg_1$	$C4/amg_1$
			$2_1/g$		bb
126	D_{4h}^4	$P4/nnc$	$P4/n\ 2/n\ 2/c$	$C4/ecg_2$	$C4/acg_2$
			$2_1/n$		bn
127	D_{4h}^5	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$	$C4/mmg_1$	$C4/mmg_1$
			$2_1/g$		nb
128	D_{4h}^6	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$	$C4/mcg_2$	$C4/mcg_2$
			$2_1/n$		nn
129	D_{4h}^7	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$	$C4/emm$	$C4amm$
			$2_1/g$		bb
130	D_{4h}^8	$P4/ncc$	$P4/n\ 2_1/c\ 2/c$	$C4/ecc$	$C4/acc$
			$2_1/n$		bn
131	D_{4h}^9	$P4_2/mmc$	$P4_2/m\ 2/m\ 2/c$	$C4_2/mcm$	$C4_2/mcm$
			$2_1/n$		nn
132	D_{4h}^{10}	$P4_2/mcm$	$P4_2/m\ 2/c\ 2/m$	$C4_2/mmc$	$C4_2/mmc$
			$2_1/g$		nb
133	D_{4h}^{11}	$P4_2/nbc$	$P4_2/n\ 2/b\ 2/c$	$C4_2/ecg_1$	$C4_2/acg_1$
			$2_1/n$		bn
134	D_{4h}^{12}	$P4_2/nnm$	$P4_2/n\ 2/n\ 2/m$	$C4_2/emg_2$	$C4_2/amg_2$
			$2_1/g$		bb
135	D_{4h}^{13}	$P4_2/mbc$	$P4_2/m\ 2_1/b\ 2/c$	$C4_2/mcg_1$	$C4_2/mcg_1$
			$2_1/n$		nn
136	D_{4h}^{14}	$P4_2/mnm$	$P4_2/m\ 2_1/n\ 2/m$	$C4_2/mmg_2$	$C4_2/mmg_2$
			$2_1/g$		nb
137	D_{4h}^{15}	$P4_2/nmc$	$P4_2/n\ 2_1/m\ 2/c$	$C4_2/ecm$	$C4_2/acm$
			$2_1/n$		bn
138	D_{4h}^{16}	$P4_2/ncm$	$P4_2/n\ 2_1/c\ 2/m$	$C4_2/emc$	$C4_2/amc$
			$2_1/g$		bb
139	D_{4h}^{17}	$I4/mmm$	$I4/m\ 2/m\ 2/m$	$F4/mmm$	$F4/mmm$
			$4_2/n\ 2_1/n\ 2_1/c$		$4_2/acg_2$
140	D_{4h}^{18}	$I4/mcm$	$I4/m\ \ 2/c\ \ 2/c$	$F4/mmc$	$F4/mcc$
			$4_2/n\ \ 2_1/b\ \ 2_1/m$		$4_2/amg_1$
141	D_{4h}^{19}	$I4_1/amd$	$I4_1/a\ \ 2/m\ \ 2/d$	$F4_1/ddm$	$F4_1/ddm$
			$4_3/b\ \ 2_1/n\ \ 2_1/d$		$4_3/ddg_2$
142	D_{4h}^{20}	$I4_1/acd$	$I4_1/a\ \ 2/c\ \ 2/d$	$F4_1/ddc$	$F4_1/ddc$
			$4_3/b\ \ 2_1/b\ \ 2_1/d$		$4_3/ddg_1$

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 P or R			Triple cell H
		Short	Full	Extended	
143	C_3^1	$P3$			$H3$
144	C_3^2	$P3_1$			$H3_1$
145	C_3^3	$P3_2$			$H3_2$
146	C_3^4	$R3$		$R3$	
				$3_{1,2}$	
147	C_{3i}^1	$P\bar{3}$			$H\bar{3}$
148	C_{3i}^2	$R\bar{3}$		$R\bar{3}$	
				$3_{1,2}$	
149	D_3^1	$P312$		$P312$	$H321$
				2_1	
150	D_3^2	$P321$		$P321$	$H312$
				2_1	
151	D_3^3	$P3_112$		$P3_112$	$H3_121$
				2_1	

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P or R			Triple cell H
		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	$P3m1$		$P3m1$ b	$H31m$
157	C_{3v}^2	$P31m$		$P31m$ a	$H3m1$
158	C_{3v}^3	$P3c1$		$P3c1$ n	$H31c$
159	C_{3v}^4	$P31c$		$P31c$ n	$H3c1$
160	C_{3v}^5	$R3m$		$R3\ m$ $3_{1,2}b$	
161	C_{3v}^6	$R3c$		$R3\ c$ $3_{1,2}n$	
162	D_{3d}^1	$P\bar{3}1m$	$P\bar{3}12/m$	$P\bar{3}12/m$ $2_1/a$	$H\bar{3}m1$
163	D_{3d}^2	$P\bar{3}1c$	$P\bar{3}12/c$	$P\bar{3}12/c$ $2_1/n$	$H\bar{3}c1$
164	D_{3d}^3	$P\bar{3}m1$	$P\bar{3}2/m1$	$P\bar{3}2/m1$ $2_1/b$	$H\bar{3}1m$
165	D_{3d}^4	$P\bar{3}c1$	$P\bar{3}2/c1$	$P\bar{3}2/c1$ $2_1/n$	$H\bar{3}1c$
166	D_{3d}^5	$R\bar{3}m$	$R\bar{3}2/m$	$R\bar{3}\ 2/m$ $3_{1,2}2_1/b$	
167	D_{3d}^6	$R\bar{3}c$	$R\bar{3}2/c$	$R\bar{3}\ 2/c$ $3_{1,2}2_1/n$	

HEXAGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P			Triple cell H
		Short	Full	Extended	
168	C_6^1	$P6$			$H6$
169	C_6^2	$P6_1$			$H6_1$
170	C_6^3	$P6_5$			$H6_5$
171	C_6^4	$P6_2$			$H6_2$
172	C_6^5	$P6_4$			$H6_4$
173	C_6^6	$P6_3$			$H6_3$
174	C_{3h}^1	$P\bar{6}$			$H\bar{6}$
175	C_{6h}^1	$P6/m$			$H6/m$
176	C_{6h}^2	$P6_3/m$			$H6_3/m$
177	D_6^1	$P622$		$P62\ 2$ 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	$H6_322$

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	*P*6*mm*		*P*6*mm* *b a*	*H*6*mm*
184	C_{6v}^2	*P*6*cc*		*P*6*cc* *nn*	*H*6*cc*
185	C_{6v}^3	$P6_3cm$		$P6_3cm$ *na*	$H6_3mc$
186	C_{6v}^4	$P6_3mc$		$P6_3mc$ *b n*	$H6_3cm$
187	D_{3h}^1	$P\bar{6}m2$		$P\bar{6}m2$ $b\,2_1$	$H\bar{6}2m$
188	D_{3h}^2	$P\bar{6}c2$		$P\bar{6}c2$ $n2_1$	$H\bar{6}2c$
189	D_{3h}^3	$P\bar{6}2m$		$P\bar{6}2m$ 2_1a	$H\bar{6}m2$
190	D_{3h}^4	$P\bar{6}2c$		$P\bar{6}2\ c$ 2_1n	$H\bar{6}c2$
191	D_{6h}^1	*P*6/*mmm*	*P*6/*m* 2/*m*2/*m*	*P*6/*m* 2/*m* 2/*m* $2_1/b$ $2_1/a$	*H*6/*mmm*
192	D_{6h}^2	*P*6/*mcc*	*P*6/*m* 2/*c* 2/*c*	*P*6/*m* 2/*c* 2/*c* $2_1/n$ $2_1/n$	*H*6/*mcc*
193	D_{6h}^3	$P6_3/mcm$	$P6_3/m\,2/c\,2/m$	$P6_3/m$ 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	*P*23		
196	T^2	*F*23		*F*23 2 2_1 2_1
197	T^3	*I*23		*I*23 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	$Pa\bar{3}$‡	$P2_1/a\bar{3}$‡	
206	T_h^7	$Ia\bar{3}$	$I2_1/a\bar{3}$	$I2_1/a\,\bar{3}$ 2/*b*
207	O^1	*P*432		*P*432 2_1
208	O^2	$P4_232$		$P4_232$ 2_1

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_22_1 4_22_1
210	O^4	$F4_132$		$F4_132$ $4_1\ 2$ $4_3\ 2_1$ $4_3\ 2_1$
211	O^5	$I432$		$I432$ $4_2\ 2_1$
212	O^6	$P4_332$		$P4_332$ 2_1
213	O^7	$P4_132$		$P4_132$ 2_1
214	O^8	$I4_132$		$I4_132$ $4_3\ 2_1$
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	$Fm\bar{3}m$	$F4/m\,\bar{3}2/m$	$F4/m\,\bar{3}\,2/m$ $4/n\quad 2/g$ $4_2/b\quad 2_1/g_2$ $4_2/a\quad 2_1/g_2$
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 $g_2(\frac{1}{4},\frac{1}{4},\frac{1}{2})$.

primitive lattice. In *Fmm*2 (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 *Pmm*2. However, in space groups *Fdd*2 (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 *Fdd*2 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 $P4_2/n\,2/b\,2/c$ (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:

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

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 $[001]_{\rm hex}$ and $[100]_{\rm hex}$, 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 $\langle 100\rangle$ and tertiary $\langle 1\bar{1}0\rangle$ 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

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

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 **a** and **b**. There are altogether six possible such multiple cells rotated by ±30°, ±90° and ±150° (*cf.* Table 1.5.1.1 and Fig. 1.5.1.8).

The hexagonal lattice is frequently referred to the orthohexagonal *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.

References

Chattopadhyay, T. K., Boucherle, J. X. & von Schnering, H. G. (1987). *Neutron diffraction study on the structural phase transition in GeTe*. *J. Phys. C*, **20**, 1431–1440.

Inorganic Crystal Structure Database (2012). Release 2012/2. Fachinformationszentrum Karlsruhe and National Institute of Standards and Technology. http://www.fiz-karlsruhe.de/icsd.html. (Abbreviated as ICSD.)

International Tables for Crystallography (1983). Vol. A, *Space-Group Symmetry*. Edited by Th. Hahn. Dordrecht: D. Reidel Publishing Company.

International Tables for Crystallography (1995). Vol. A, *Space-Group Symmetry*. Edited by Th. Hahn, 4th revised ed. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2002). Vol. A, *Space-Group Symmetry*. Edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2010). Vol. A1, *Symmetry Relations between Space Groups*. Edited by H. Wondratschek & U. Müller, 2nd ed. Chichester: John Wiley & Sons.

International Tables for X-ray Crystallography (1952). Vol. I, *Symmetry Groups*, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press.

Krstanovic, I. R. (1958). *Redetermination of the oxygen parameters in zircon ($ZrSiO_4$)*. *Acta Cryst.* **11**, 896–897.

Wiedemeier, H. & Siemers, P. A. (1989). *The thermal expansion of GeS and GeTe*. *J. Less Common Met.* **146**, 279–298.

Wolff, P. M. de, Billiet, Y., Donnay, J. D. H., Fischer, W., Galiulin, R. B., Glazer, A. M., Hahn, Th., Senechal, M., Shoemaker, D. P., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1992). *Symbols for symmetry elements and symmetry operations. Final Report of the International Union of Crystallography Ad-hoc Committee on the Nomenclature of Symmetry*. *Acta Cryst.* A**48**, 727–732.

Wyckoff, R. W. G. & Hendricks, S. B. (1927). *Die Kristallstruktur von Zirkon und die Kriterien fuer spezielle Lagen in tetragonalen Raumgruppen*. *Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem.* **66**, 73–102.