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)

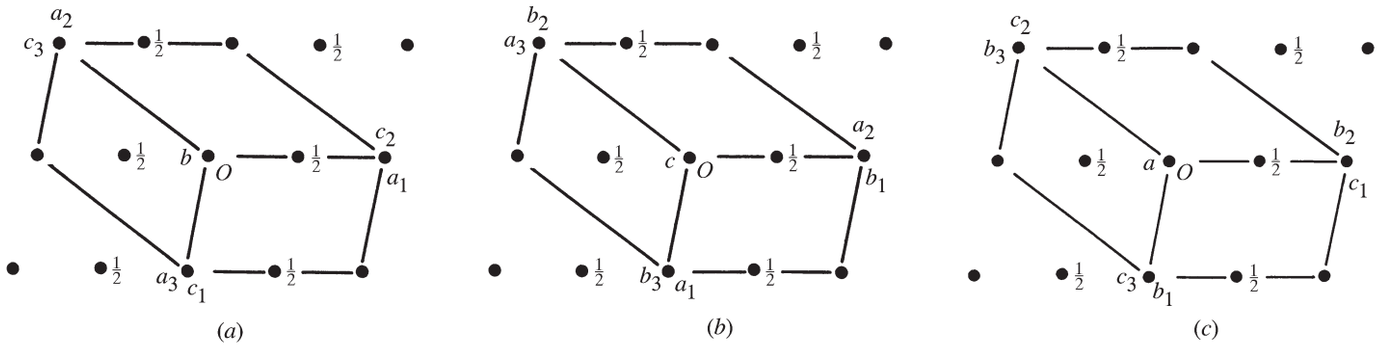


Figure 1.5.1.2
Monoclinic centred lattice, projected along the unique axis. The origin for all the cells is the same. The fractions $\frac{1}{2}$ indicate the height of the lattice points along the axis of projection.

(*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.

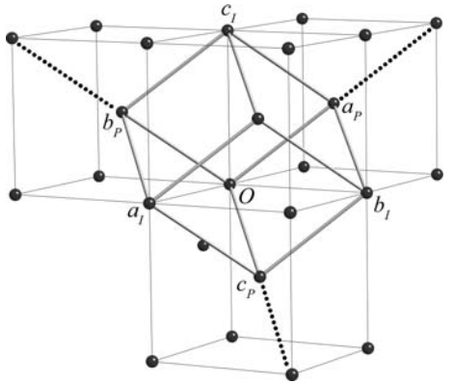


Figure 1.5.1.3
Body-centred cell *I* with a_I, b_I, c_I and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *I* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{3}$ and $\alpha =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

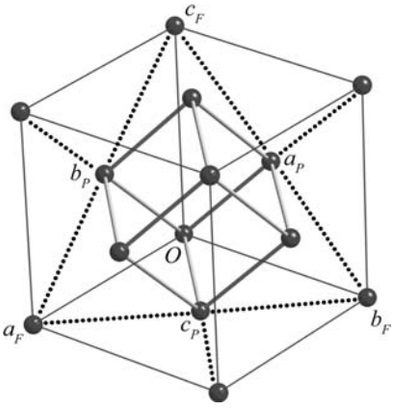


Figure 1.5.1.4
Face-centred cell *F* with a_F, b_F, c_F and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *F* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{2}$ and $\alpha =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

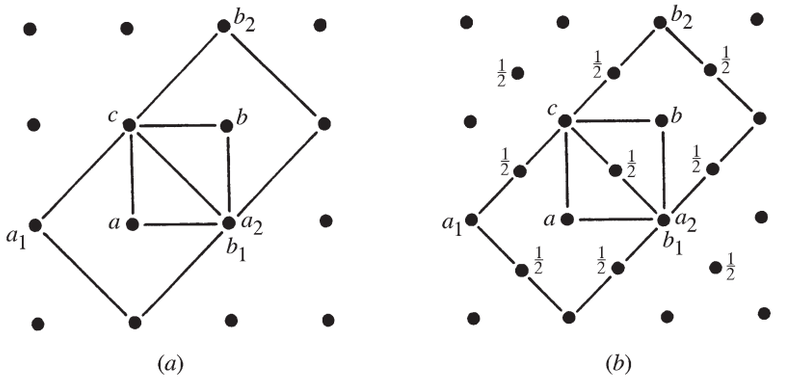


Figure 1.5.1.5
Tetragonal lattices, projected along $[00\bar{1}]$. (*a*) Primitive cell P with a, b, c and the C-centred cells C_1 with a_1, b_1, c and C_2 with a_2, b_2, c. The origin for all three cells is the same. (*b*) Body-centred cell I with a, b, c and the F-centred cells F_1 with a_1, b_1, c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

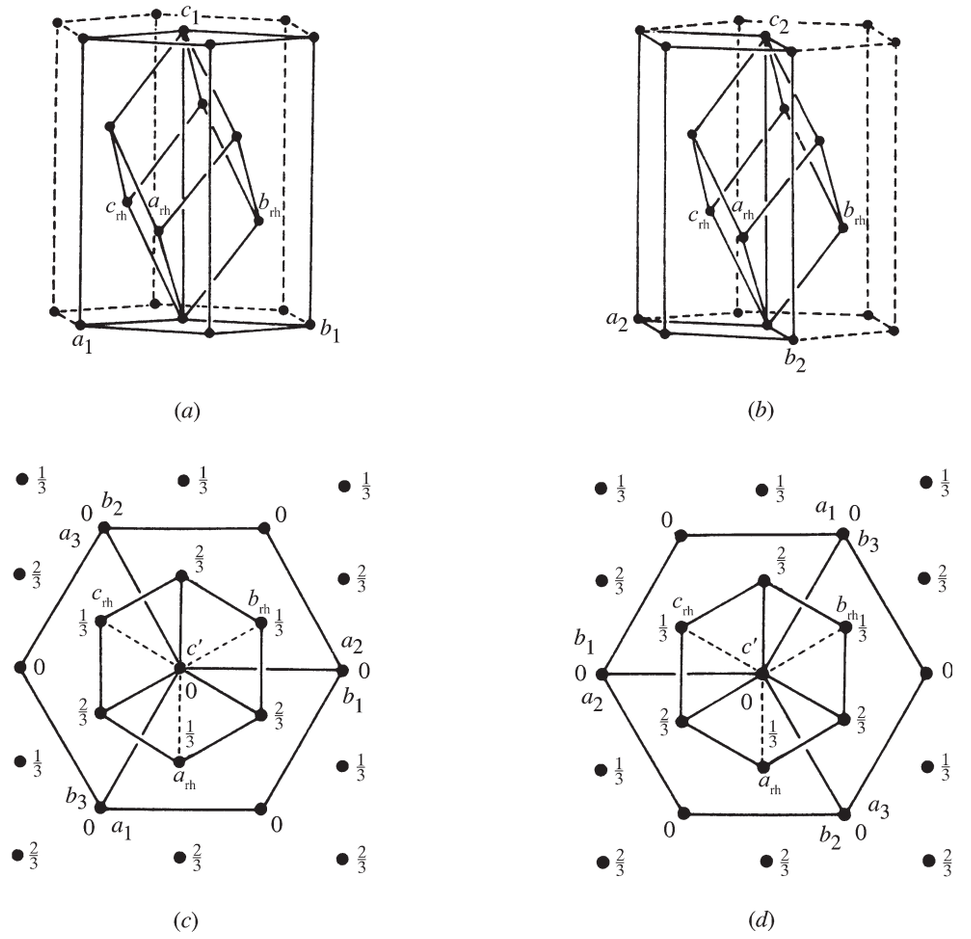


Figure 1.5.1.6
Unit cells in the rhombohedral lattice: same origin for all cells. The basis of the rhombohedral cell is labelled a_{rh}, b_{rh}, c_{rh}. Two settings of the triple hexagonal cell are possible with respect to a primitive rhombohedral cell: The *obverse setting* with the lattice points 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'.

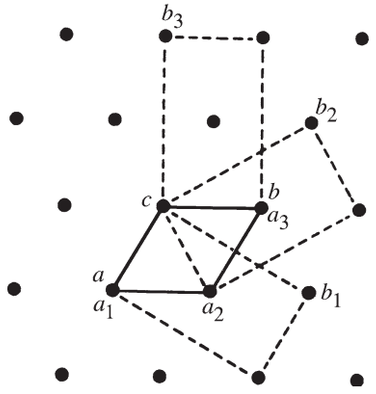


Figure 1.5.1.7
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three C-centred (orthohexagonal) cells a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.

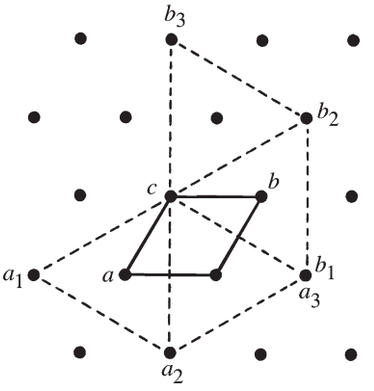
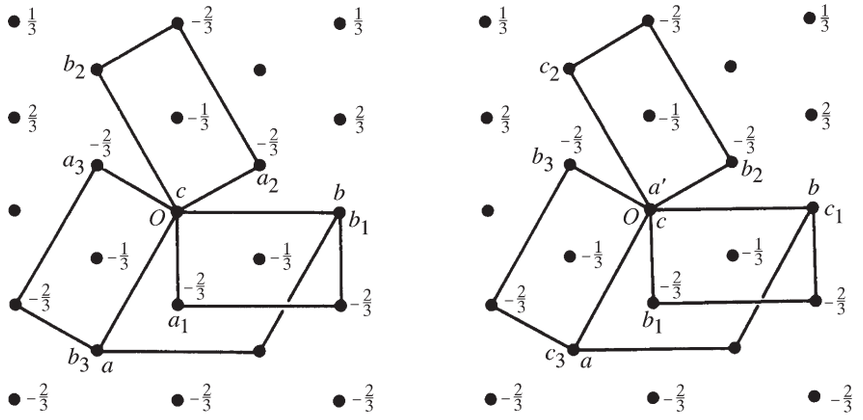
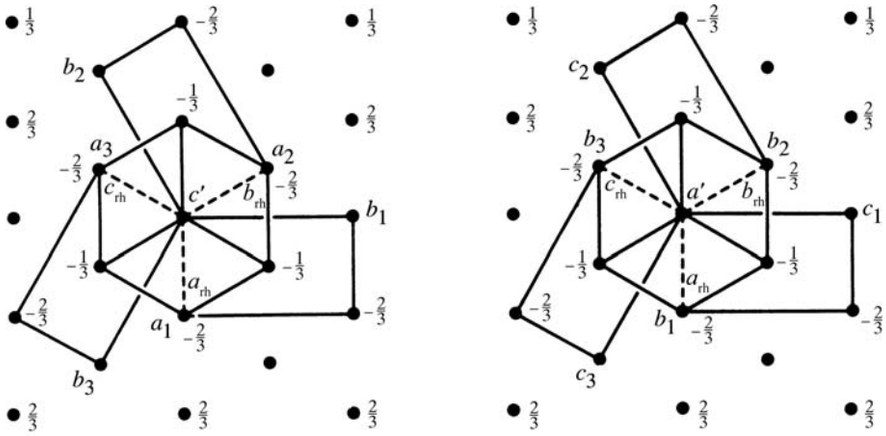


Figure 1.5.1.8
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three triple hexagonal cells H with a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.



(*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.*

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:

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

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).

1.5.2. 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 $\mathbf{a}, \mathbf{b}, \mathbf{c}$:

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

references