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 $0 \le x_i < 1$):

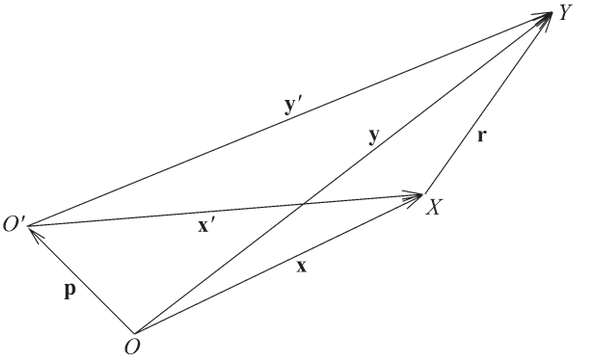


Figure 1.5.1.1
The coordinates of the points X (or Y) with respect to the old origin O are $\boldsymbol{x}$ ($\boldsymbol{y}$), and with respect to the new origin O' they are $\boldsymbol{x}'$ ($\boldsymbol{y}'$). From the diagram one reads $\mathbf{p} + \mathbf{x}' = \mathbf{x}$ and $\mathbf{p} + \mathbf{y}'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

[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)

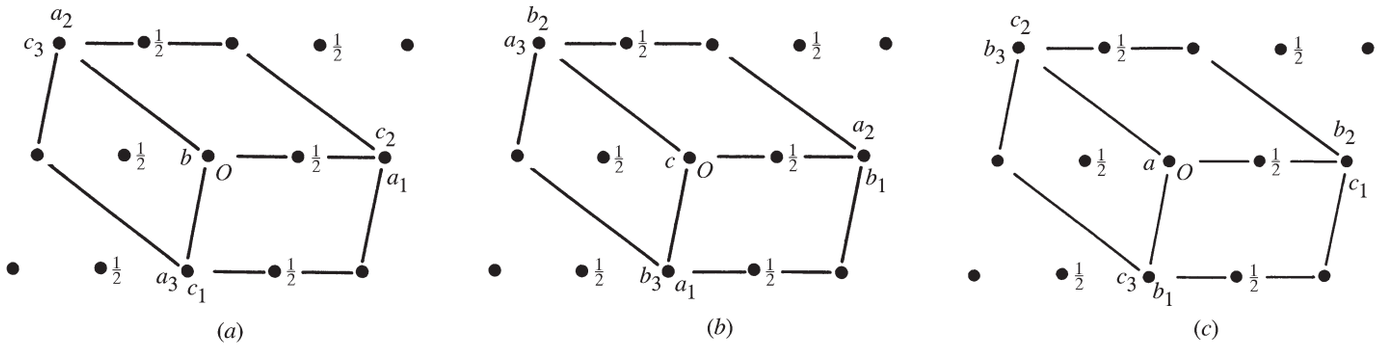


Figure 1.5.1.2
Monoclinic centred lattice, projected along the unique axis. The origin for all the cells is the same. The fractions $\frac{1}{2}$ indicate the height of the lattice points along the axis of projection.

(*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.

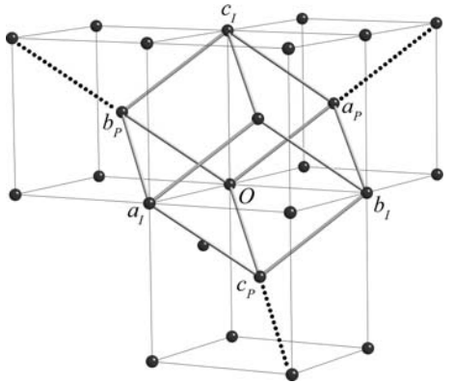


Figure 1.5.1.3
Body-centred cell *I* with a_I, b_I, c_I and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *I* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{3}$ and $\alpha =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

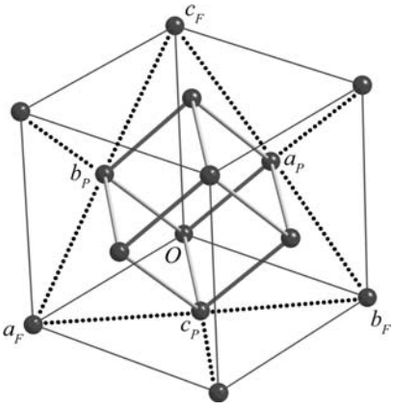


Figure 1.5.1.4
Face-centred cell *F* with a_F, b_F, c_F and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *F* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{2}$ and $\alpha =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

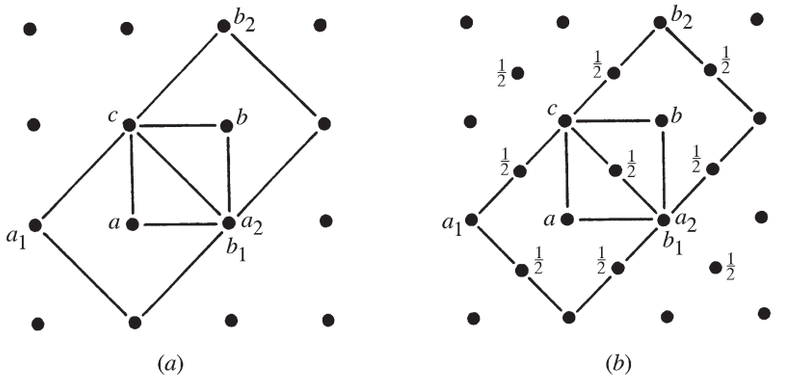


Figure 1.5.1.5
Tetragonal lattices, projected along $[00\bar{1}]$. (*a*) Primitive cell P with a, b, c and the C-centred cells C_1 with a_1, b_1, c and C_2 with a_2, b_2, c. The origin for all three cells is the same. (*b*) Body-centred cell I with a, b, c and the F-centred cells F_1 with a_1, b_1, c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

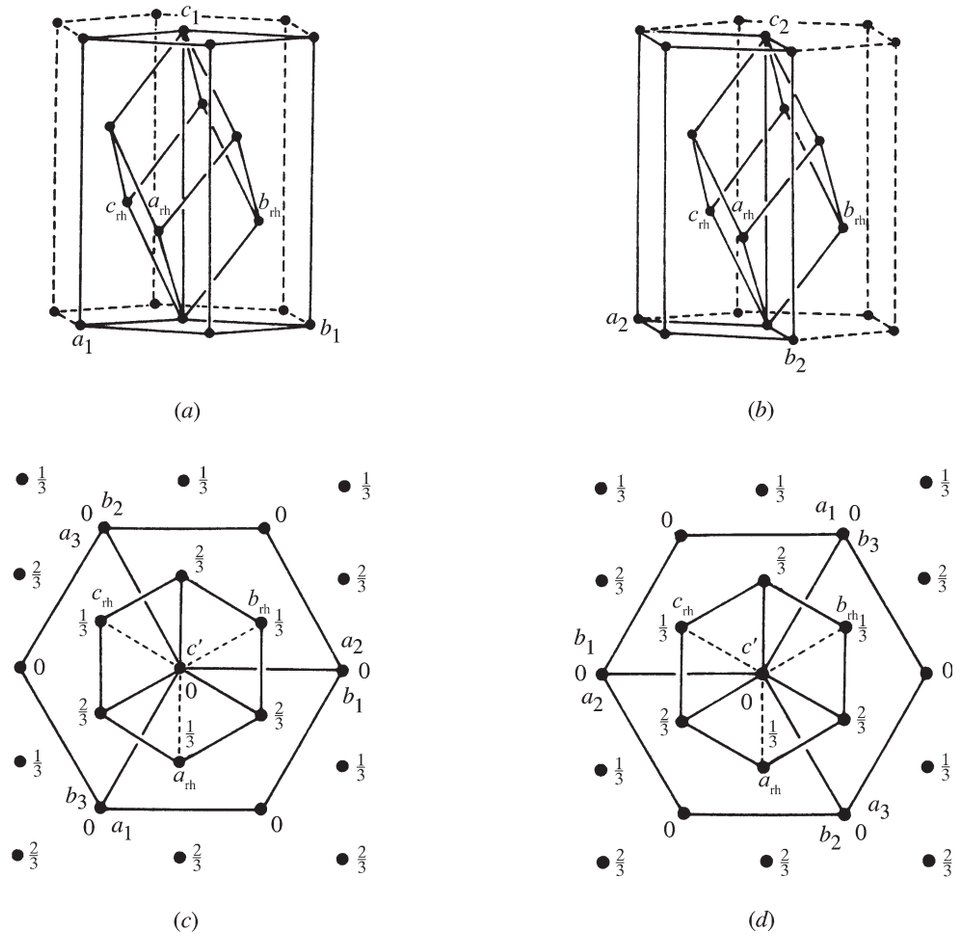


Figure 1.5.1.6
Unit cells in the rhombohedral lattice: same origin for all cells. The basis of the rhombohedral cell is labelled a_{rh}, b_{rh}, c_{rh}. Two settings of the triple hexagonal cell are possible with respect to a primitive rhombohedral cell: The *obverse setting* with the lattice points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

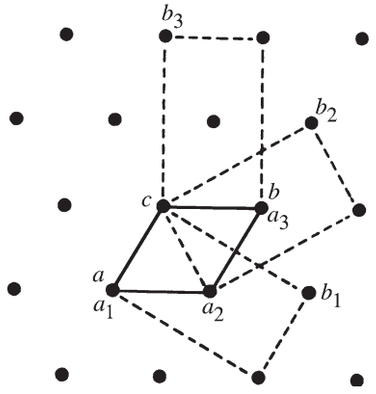


Figure 1.5.1.7
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three C-centred (orthohexagonal) cells a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.

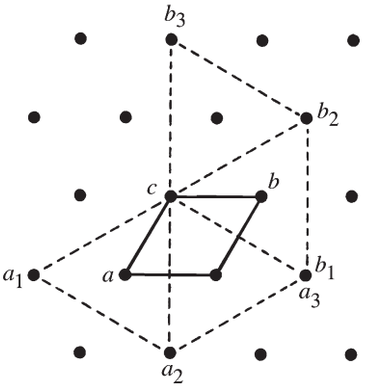
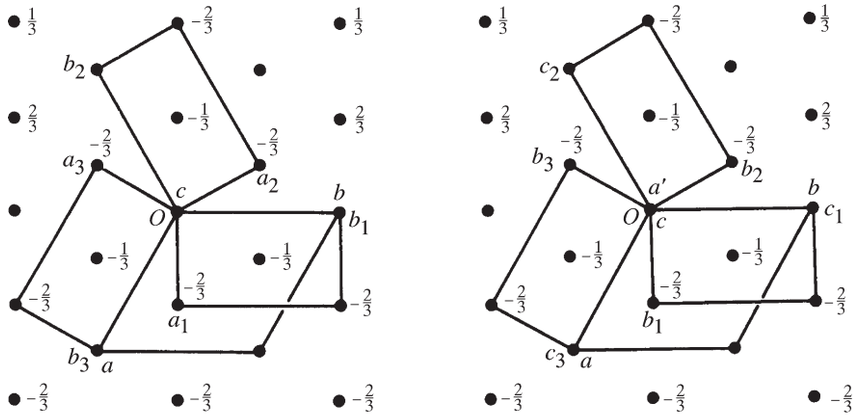
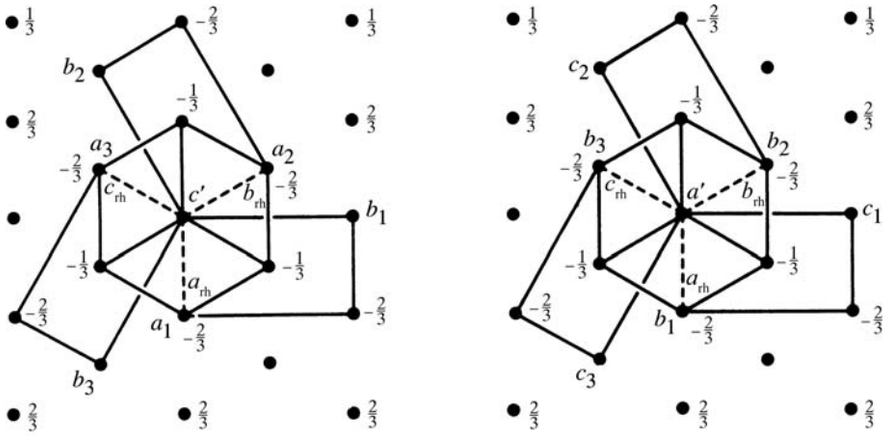


Figure 1.5.1.8
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three triple hexagonal cells H with a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.



(*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.*

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

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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