International Tables for Crystallography (2006). Vol. A, Chapter 5.1, pp. 78–85.

5.1. Transformations of the coordinate system (unit-cell transformations)

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5.1.1. Introduction

There are two main uses of transformations in crystallography.

(i) *Transformation of the coordinate system* and the unit cell while keeping the crystal at rest. This aspect forms the main topic of the present part. Transformations of coordinate systems are useful when nonconventional descriptions of a crystal structure are considered, for instance in the study of relations between different structures, of phase transitions and of group–subgroup relations. Unit-cell transformations occur particularly frequently when different settings or cell choices of monoclinic, orthorhombic or rhombohedral space groups are to be compared or when 'reduced cells' are derived.

(ii) Description of the *symmetry operations* (motions) of an object (crystal structure). This involves the transformation of the coordinates of a point or the components of a position vector while keeping the coordinate system unchanged. Symmetry operations are treated in Chapter 8.1 and Part 11. They are briefly reviewed in Chapter 5.2.

5.1.2. Matrix notation

Throughout this volume, matrices are written in the following notation:

As (1 × 3) row matrices:

(**a**, **b**, **c**)	the basis vectors of direct space
(*h*, *k*, *l*)	the Miller indices of a plane (or a set of planes) in direct space or the coordinates of a point in reciprocal space

As (3 × 1) or (4 × 1) column matrices:

$x = (x/y/z)$	the coordinates of a point in direct space
$(\mathbf{a}^*/\mathbf{b}^*/\mathbf{c}^*)$	the basis vectors of reciprocal space
$(u/v/w)$	the indices of a direction in direct space
$\boldsymbol{p} = (p_1/p_2/p_3)$	the components of a shift vector from origin O to the new origin O'
$\boldsymbol{q} = (q_1/q_2/q_3)$	the components of an inverse origin shift from origin O' to origin O, with $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$
$\boldsymbol{w} = (w_1/w_2/w_3)$	the translation part of a symmetry operation W in direct space
$\mathbb{X} = (x/y/z/1)$	the augmented (4 × 1) column matrix of the coordinates of a point in direct space

As (3 × 3) or (4 × 4) square matrices:

$\boldsymbol{P}, \boldsymbol{Q} = \boldsymbol{P}^{-1}$	linear parts of an affine transformation; if $\boldsymbol{P}$ is applied to a (1 × 3) row matrix, $\boldsymbol{Q}$ must be applied to a (3 × 1) column matrix, and *vice versa*
$\boldsymbol{W}$	the rotation part of a symmetry operation W in direct space
$\mathbb{P} = \begin{pmatrix} \boldsymbol{P} & \boldsymbol{p} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented affine (4 × 4) transformation matrix, with $\boldsymbol{o} = (0, 0, 0)$
$\mathbb{Q} = \begin{pmatrix} \boldsymbol{Q} & \boldsymbol{q} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented affine (4 × 4) transformation matrix, with $\mathbb{Q} = \mathbb{P}^{-1}$
$\mathbb{W} = \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{o} & 1 \end{pmatrix}$	the augmented (4 × 4) matrix of a symmetry operation in direct space (*cf.* Chapter 8.1 and Part 11).

5.1.3. General transformation

Here the crystal structure is considered to be at rest, whereas the coordinate system and the unit cell are changed. Specifically, a point X in a crystal is defined with respect to the basis vectors **a**, **b**, **c** and the origin O by the coordinates x, y, z, *i.e.* the position vector **r** of point X is given by

$$\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

The same point X is given with respect to a new coordinate system, *i.e.* the new basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ and the new origin O' (Fig. 5.1.3.1), by the position vector

$$\mathbf{r}' = x'\mathbf{a}' + y'\mathbf{b}' + z'\mathbf{c}'.$$

In this section, the relations between the primed and unprimed quantities are treated.

The general transformation (affine transformation) of the coordinate system consists of two parts, a linear part and a shift of origin. The (3 × 3) matrix $\boldsymbol{P}$ of the linear part and the (3 × 1) column matrix $\boldsymbol{p}$, containing the components of the shift vector $\boldsymbol{p}$, define the transformation uniquely. It is represented by the symbol $(\boldsymbol{P}, \boldsymbol{p})$.

(i) The *linear part* implies a change of orientation or length or both of the basis vectors **a**, **b**, **c**, *i.e.*

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

For a pure linear transformation, the shift vector **p** is zero and the symbol is $(\boldsymbol{P}, \boldsymbol{o})$.

The determinant of $\boldsymbol{P}$, $\det(\boldsymbol{P})$, should be positive. If $\det(\boldsymbol{P})$ is negative, a right-handed coordinate system is transformed into a left-handed one (or *vice versa*). If $\det(\boldsymbol{P}) = 0$, the new basis vectors are linearly dependent and do not form a complete coordinate system.

In this chapter, transformations in three-dimensional space are treated. A change of the basis vectors in two dimensions, *i.e.* of the basis vectors **a** and **b**, can be considered as a three-dimensional transformation with invariant **c** axis. This is achieved by setting $P_{33} = 1$ and $P_{13} = P_{23} = P_{31} = P_{32} = 0$.

(ii) A *shift of origin* is defined by the shift vector

$$\mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}.$$

The basis vectors **a**, **b**, **c** are fixed at the origin O; the new basis vectors are fixed at the new origin O' which has the coordinates p_1, p_2, p_3 in the old coordinate system (Fig. 5.1.3.1).

For a pure origin shift, the basis vectors do not change their lengths or orientations. In this case, the transformation matrix $\boldsymbol{P}$ is the unit matrix $\boldsymbol{I}$ and the symbol of the pure shift becomes $(\boldsymbol{I}, \boldsymbol{p})$.

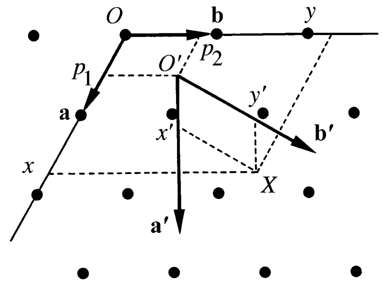


Fig. 5.1.3.1. General affine transformation, consisting of a shift of origin from O to O' by a shift vector $\mathbf{p}$ with components p_1 and p_2 and a change of basis from $\mathbf{a}$, $\mathbf{b}$ to $\mathbf{a}'$, $\mathbf{b}'$. This implies a change in the coordinates of the point X from x, y to x', y'.

Also, the inverse matrices of $\boldsymbol{P}$ and $\boldsymbol{p}$ are needed. They are

$$\boldsymbol{Q} = \boldsymbol{P}^{-1}$$

and

$$\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}.$$

The matrix $\boldsymbol{q}$ consists of the components of the negative shift vector $\mathbf{q}$ which refer to the coordinate system $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$, *i.e.*

$$\mathbf{q} = q_1\mathbf{a}' + q_2\mathbf{b}' + q_3\mathbf{c}'.$$

Thus, the transformation ($\boldsymbol{Q}$, $\boldsymbol{q}$) is the inverse transformation of ($\boldsymbol{P}$, $\boldsymbol{p}$). Applying ($\boldsymbol{Q}$, $\boldsymbol{q}$) to the basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ and the origin O', the old basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ with origin O are obtained.

For a two-dimensional transformation of $\mathbf{a}'$ and $\mathbf{b}'$, some elements of $\boldsymbol{Q}$ are set as follows: $Q_{33} = 1$ and $Q_{13} = Q_{23} = Q_{31} = Q_{32} = 0$.

The quantities which transform in the same way as the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are called *covariant* quantities and are written as row matrices. They are:

the *Miller indices of a plane* (or a set of planes), (hkl), in direct space and

the *coordinates of a point in reciprocal space*, h, k, l.

Both are transformed by

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

Usually, the Miller indices are made relative prime before and after the transformation.

The quantities which are covariant with respect to the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are *contravariant* with respect to the basis vectors $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ of reciprocal space.

The *basis vectors of reciprocal space* are written as a column matrix and their transformation is achieved by the matrix $\boldsymbol{Q}$:

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

The inverse transformation is obtained by the inverse matrix $\boldsymbol{P} = \boldsymbol{Q}^{-1}$:

$$\begin{pmatrix} \mathbf{a}^{*} \\ \mathbf{b}^{*} \\ \mathbf{c}^{*} \end{pmatrix} = \boldsymbol{P} \begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix}.$$

These transformation rules apply also to the quantities covariant with respect to the basis vectors $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ and contravariant with respect to $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, which are written as column matrices. They are the *indices of a direction* in direct space, [uvw], which are transformed by

$$\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = \boldsymbol{Q} \begin{pmatrix} u \\ v \\ w \end{pmatrix}.$$

In contrast to all quantities mentioned above, the *components of a position vector* $\mathbf{r}$ or the *coordinates of a point X in direct space* x, y, z depend also on the shift of the origin in direct space. The general (affine) transformation is given by

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \boldsymbol{Q} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \boldsymbol{q} = \begin{pmatrix} Q_{11}x + Q_{12}y + Q_{13}z + q_1 \\ Q_{21}x + Q_{22}y + Q_{23}z + q_2 \\ Q_{31}x + Q_{32}y + Q_{33}z + q_3 \end{pmatrix}.$$

Example

If no shift of origin is applied, *i.e.* $\boldsymbol{p} = \boldsymbol{q} = \boldsymbol{o}$, the position vector $\mathbf{r}$ of point X is transformed by

$$\mathbf{r}' = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}\boldsymbol{Q} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = (\mathbf{a}', \mathbf{b}', \mathbf{c}') \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}.$$

In this case, $\mathbf{r} = \mathbf{r}'$, *i.e.* the position vector is invariant, although the basis vectors and the components are transformed. For a pure shift of origin, *i.e.* $\boldsymbol{P} = \boldsymbol{Q} = \boldsymbol{I}$, the transformed position vector $\mathbf{r}'$ becomes

$$\begin{aligned} \mathbf{r}' &= (x + q_1)\mathbf{a} + (y + q_2)\mathbf{b} + (z + q_3)\mathbf{c} \\ &= \mathbf{r} + q_1\mathbf{a} + q_2\mathbf{b} + q_3\mathbf{c} \\ &= (x - p_1)\mathbf{a} + (y - p_2)\mathbf{b} + (z - p_3)\mathbf{c} \\ &= \mathbf{r} - p_1\mathbf{a} - p_2\mathbf{b} - p_3\mathbf{c}. \end{aligned}$$

Here the transformed vector $\mathbf{r}'$ is no longer identical with $\mathbf{r}$.

It is convenient to introduce the augmented (4×4) matrix $\mathbb{Q}$ which is composed of the matrices $\boldsymbol{Q}$ and $\boldsymbol{q}$ in the following manner (*cf.* Chapter 8.1):

$$\mathbb{Q} = \begin{pmatrix} \boldsymbol{Q} & \boldsymbol{q} \\ \boldsymbol{o} & 1 \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with $\boldsymbol{o}$ the (1×3) row matrix containing zeros. In this notation, the transformed coordinates x', y', z' are obtained by

Table 5.1.3.1. *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
$\mathbf{c} \rightarrow \frac{1}{2}\mathbf{c}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$	All systems
$\mathbf{b} \rightarrow \frac{1}{2}\mathbf{b}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	All systems
$\mathbf{a} \rightarrow \frac{1}{2}\mathbf{a}$	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	All systems
Cell choice 1 → cell choice 2: $\begin{cases} P \rightarrow P \\ C \rightarrow A \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \rightarrow P \\ A \rightarrow I \end{cases}$ Unique axis **b** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \rightarrow P \\ I \rightarrow C \end{cases}$ (Fig. 5.1.3.2*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.* Section 2.2.16)
Cell choice 1 → cell choice 2: $\begin{cases} P \rightarrow P \\ A \rightarrow B \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \rightarrow P \\ B \rightarrow I \end{cases}$ Unique axis **c** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \rightarrow P \\ I \rightarrow A \end{cases}$ (Fig. 5.1.3.2*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.* Section 2.2.16)
Cell choice 1 → cell choice 2: $\begin{cases} P \rightarrow P \\ B \rightarrow C \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \rightarrow P \\ C \rightarrow I \end{cases}$ Unique axis **a** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \rightarrow P \\ I \rightarrow B \end{cases}$ (Fig. 5.1.3.2*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.* Section 2.2.16)
Unique axis **b** → unique axis **c** Cell choice 1: $\begin{cases} P \rightarrow P \\ C \rightarrow A \end{cases}$ Cell choice 2: $\begin{cases} P \rightarrow P \\ A \rightarrow B \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \rightarrow P \\ I \rightarrow I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
Unique axis **b** → unique axis **a** Cell choice 1: $\begin{cases} P \rightarrow P \\ C \rightarrow B \end{cases}$ Cell choice 2: $\begin{cases} P \rightarrow P \\ A \rightarrow C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \rightarrow P \\ I \rightarrow I \end{cases}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
Unique axis **c** → unique axis **a** Cell choice 1: $\begin{cases} P \rightarrow P \\ A \rightarrow B \end{cases}$ Cell choice 2: $\begin{cases} P \rightarrow P \\ B \rightarrow C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \rightarrow P \\ I \rightarrow I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Section 2.2.16)
$I \rightarrow P$ (Fig. 5.1.3.3) $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c}) \rightarrow (\mathbf{a}' + \mathbf{b}' + \mathbf{c}')$	$\begin{pmatrix} \bar{\frac{1}{2}} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \bar{\frac{1}{2}} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	Orthorhombic Tetragonal Cubic

Table 5.1.3.1. *Selected 3 × 3 transformation matrices* $\boldsymbol{P}$ *and* $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ (*cont.*)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
$F \rightarrow P$ (Fig. 5.1.3.4) ($\mathbf{a}+\mathbf{b}+\mathbf{c}$) invariant vector	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	Orthorhombic Tetragonal Cubic
$(\mathbf{b}, \mathbf{a}, \bar{\mathbf{c}}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	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
$\left.\begin{matrix} P \rightarrow C_1 \\ I \rightarrow F_1 \end{matrix}\right\}$ (Fig. 5.1.3.5) **c** axis invariant	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\bar{1}}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 4.3.4)
$\left.\begin{matrix} P \rightarrow C_2 \\ I \rightarrow F_2 \end{matrix}\right\}$ (Fig. 5.1.3.5) **c** axis invariant	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 4.3.4)
Primitive rhombohedral cell → triple hexagonal cell R_1, obverse setting (Fig. 5.1.3.6*c*)	$\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \frac{\bar{1}}{3} & \frac{\bar{1}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{\bar{2}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_2, obverse setting (Fig. 5.1.3.6*c*)	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 1 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{3} & \frac{2}{3} & \frac{\bar{1}}{3} \\ \frac{\bar{2}}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_3, obverse setting (Fig. 5.1.3.6*c*)	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{3} & \frac{\bar{1}}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{\bar{2}}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_1, reverse setting (Fig. 5.1.3.6*d*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \\ 0 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{2}}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{\bar{1}}{3} & \frac{\bar{1}}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_2, reverse setting (Fig. 5.1.3.6*d*)	$\begin{pmatrix} 0 & 1 & 1 \\ \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{\bar{2}}{3} & \frac{1}{3} \\ \frac{2}{3} & \frac{\bar{1}}{3} & \frac{\bar{1}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → triple hexagonal cell R_3, reverse setting (Fig. 5.1.3.6*d*)	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{\bar{2}}{3} \\ \frac{\bar{1}}{3} & \frac{2}{3} & \frac{\bar{1}}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Hexagonal cell P → orthohexagonal centred cell C_1 (Fig. 5.1.3.7)	$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \frac{\bar{1}}{2} & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → orthohexagonal centred cell C_2 (Fig. 5.1.3.7)	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{\bar{1}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → orthohexagonal centred cell C_3 (Fig. 5.1.3.7)	$\begin{pmatrix} 0 & \bar{2} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{\bar{1}}{2} & 1 & 0 \\ \frac{\bar{1}}{2} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)

Table 5.1.3.1. *Selected 3 × 3 transformation matrices **P** and **Q** = **P**$^{-1}$* (*cont.*)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q}=\boldsymbol{P}^{-1}$	Crystal system
Hexagonal cell P → triple hexagonal cell H_1 (Fig. 5.1.3.8)	$\begin{pmatrix}1&1&0\\ \bar{1}&2&0\\ 0&0&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{2}{3}&\tfrac{\bar{1}}{3}&0\\ \tfrac{1}{3}&\tfrac{1}{3}&0\\ 0&0&1\end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple hexagonal cell H_2 (Fig. 5.1.3.8)	$\begin{pmatrix}2&\bar{1}&0\\ 1&1&0\\ 0&0&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{1}{3}&\tfrac{1}{3}&0\\ \tfrac{\bar{1}}{3}&\tfrac{2}{3}&0\\ 0&0&1\end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple hexagonal cell H_3 (Fig. 5.1.3.8)	$\begin{pmatrix}1&\bar{2}&0\\ 2&\bar{1}&0\\ 0&0&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{\bar{1}}{3}&\tfrac{2}{3}&0\\ \tfrac{\bar{2}}{3}&\tfrac{1}{3}&0\\ 0&0&1\end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple rhombohedral cell D_1	$\begin{pmatrix}1&0&\bar{1}\\ 0&1&\bar{1}\\ 1&1&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{2}{3}&\tfrac{\bar{1}}{3}&\tfrac{1}{3}\\ \tfrac{\bar{1}}{3}&\tfrac{2}{3}&\tfrac{1}{3}\\ \tfrac{\bar{1}}{3}&\tfrac{\bar{1}}{3}&\tfrac{1}{3}\end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Hexagonal cell P → triple rhombohedral cell D_2	$\begin{pmatrix}\bar{1}&0&1\\ 0&\bar{1}&1\\ 1&1&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{\bar{2}}{3}&\tfrac{1}{3}&\tfrac{1}{3}\\ \tfrac{1}{3}&\tfrac{\bar{2}}{3}&\tfrac{1}{3}\\ \tfrac{1}{3}&\tfrac{1}{3}&\tfrac{1}{3}\end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 5.1.3.9*a*) **c** and **b** axes invariant	$\begin{pmatrix}\tfrac{2}{3}&0&0\\ \tfrac{1}{3}&1&0\\ \tfrac{\bar{2}}{3}&0&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{3}{2}&0&0\\ \tfrac{\bar{1}}{2}&1&0\\ 1&0&1\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 5.1.3.9*a*) **c** axis invariant	$\begin{pmatrix}\tfrac{\bar{1}}{3}&\bar{1}&0\\ \tfrac{1}{3}&\bar{1}&0\\ \tfrac{\bar{2}}{3}&0&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{\bar{3}}{2}&\tfrac{3}{2}&0\\ \tfrac{\bar{1}}{2}&\tfrac{\bar{1}}{2}&0\\ \bar{1}&1&1\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → C-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 5.1.3.9*a*) $\mathbf{a}_{\rm h}\to\mathbf{b}_{\rm m}$, **c** axis invariant	$\begin{pmatrix}\tfrac{\bar{1}}{3}&1&0\\ \tfrac{\bar{2}}{3}&0&0\\ \tfrac{\bar{2}}{3}&0&1\end{pmatrix}$	$\begin{pmatrix}0&\tfrac{\bar{3}}{2}&0\\ 1&\tfrac{\bar{1}}{2}&0\\ 0&\bar{1}&1\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → A-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig. 5.1.3.9*b*) $\mathbf{b}_{\rm h}\to\mathbf{c}_{\rm m}, \mathbf{c}_{\rm h}\to\mathbf{a}_{\rm m}$	$\begin{pmatrix}0&\tfrac{2}{3}&0\\ 0&\tfrac{1}{3}&1\\ 1&\tfrac{\bar{2}}{3}&0\end{pmatrix}$	$\begin{pmatrix}1&0&1\\ \tfrac{3}{2}&0&0\\ \tfrac{\bar{1}}{2}&1&0\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → A-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 5.1.3.9*b*) $\mathbf{c}_{\rm h}\to\mathbf{a}_{\rm m}$	$\begin{pmatrix}0&\tfrac{\bar{1}}{3}&\bar{1}\\ 0&\tfrac{1}{3}&\bar{1}\\ 1&\tfrac{\bar{2}}{3}&0\end{pmatrix}$	$\begin{pmatrix}\bar{1}&1&1\\ \tfrac{\bar{3}}{2}&\tfrac{3}{2}&0\\ \tfrac{\bar{1}}{2}&\tfrac{\bar{1}}{2}&0\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Triple hexagonal cell R, obverse setting → A-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 5.1.3.9*b*) $\mathbf{a}_{\rm h}\to\mathbf{c}_{\rm m}, \mathbf{c}_{\rm h}\to\mathbf{a}_{\rm m}$	$\begin{pmatrix}0&\tfrac{\bar{1}}{3}&1\\ 0&\tfrac{\bar{2}}{3}&0\\ 1&\tfrac{\bar{2}}{3}&0\end{pmatrix}$	$\begin{pmatrix}0&\bar{1}&1\\ 0&\tfrac{\bar{3}}{2}&0\\ 1&\tfrac{\bar{1}}{2}&0\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 5.1.3.10*a*) $[111]_{\rm r}\to\mathbf{c}_{\rm m}$	$\begin{pmatrix}0&0&1\\ \bar{1}&1&1\\ \bar{1}&\bar{1}&1\end{pmatrix}$	$\begin{pmatrix}1&\tfrac{\bar{1}}{2}&\tfrac{\bar{1}}{2}\\ 0&\tfrac{1}{2}&\tfrac{\bar{1}}{2}\\ 1&0&0\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 5.1.3.10*a*) $[111]_{\rm r}\to\mathbf{c}_{\rm m}$	$\begin{pmatrix}\bar{1}&\bar{1}&1\\ 0&0&1\\ \bar{1}&1&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{\bar{1}}{2}&1&\tfrac{\bar{1}}{2}\\ \tfrac{\bar{1}}{2}&0&\tfrac{1}{2}\\ 0&1&0\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → C-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 5.1.3.10*a*) $[111]_{\rm r}\to\mathbf{c}_{\rm m}$	$\begin{pmatrix}\bar{1}&1&1\\ \bar{1}&\bar{1}&1\\ 0&0&1\end{pmatrix}$	$\begin{pmatrix}\tfrac{\bar{1}}{2}&\tfrac{\bar{1}}{2}&1\\ \tfrac{1}{2}&\tfrac{\bar{1}}{2}&0\\ 0&0&1\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → A-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig. 5.1.3.10*b*) $[111]_{\rm r}\to\mathbf{a}_{\rm m}$	$\begin{pmatrix}1&0&0\\ 1&\bar{1}&1\\ 1&\bar{1}&\bar{1}\end{pmatrix}$	$\begin{pmatrix}1&0&0\\ 1&\tfrac{\bar{1}}{2}&\tfrac{\bar{1}}{2}\\ 0&\tfrac{1}{2}&\tfrac{\bar{1}}{2}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)
Primitive rhombohedral cell → A-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 5.1.3.10*b*) $[111]_{\rm r}\to\mathbf{a}_{\rm m}$	$\begin{pmatrix}1&\bar{1}&\bar{1}\\ 1&0&0\\ 1&\bar{1}&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\ \tfrac{\bar{1}}{2}&1&\tfrac{\bar{1}}{2}\\ \tfrac{\bar{1}}{2}&0&\tfrac{1}{2}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)

Table 5.1.3.1. *Selected 3 × 3 transformation matrices* $\boldsymbol{P}$ *and* $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ (*cont.*)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 5.1.3.10*b*) $[111]_r \rightarrow \mathbf{a}_m$	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ \frac{\bar{1}}{2} & \frac{\bar{1}}{2} & 1 \\ \frac{1}{2} & \frac{\bar{1}}{2} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 4.3.5)

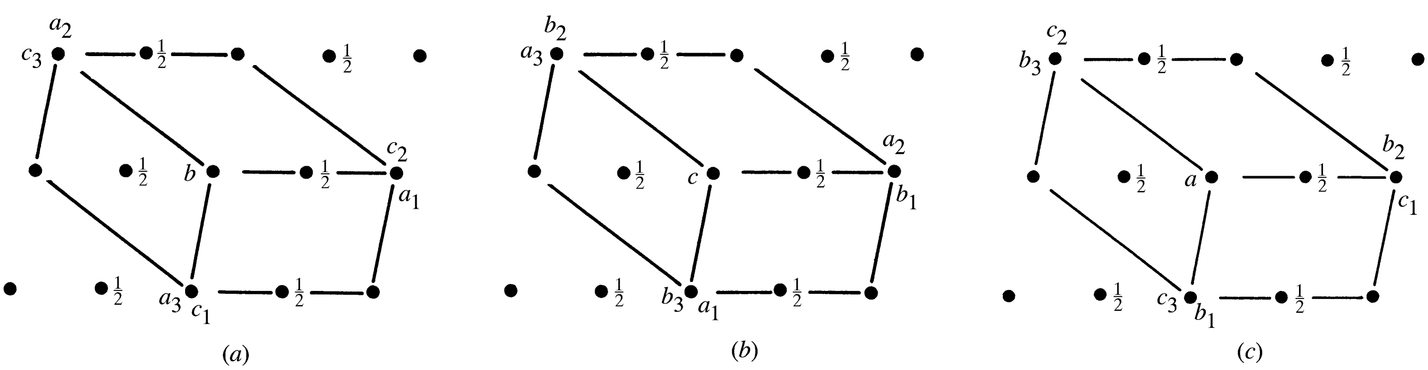


Fig. 5.1.3.2. Monoclinic centred lattice, projected along the unique axis. Origin for all cells is the same.

(*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.

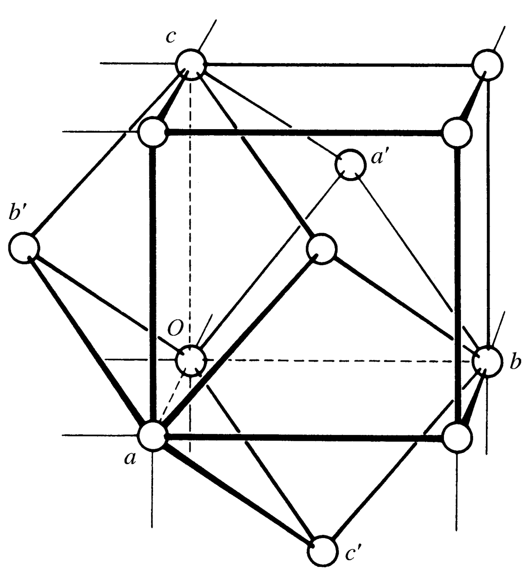


Fig. 5.1.3.3. Body-centred cell *I* with *a*, *b*, *c* and a corresponding primitive cell *P* with *a*′, *b*′, *c*′. Origin for both cells *O*. A cubic *I* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_r = a_c \frac{1}{2}\sqrt{3}$ and $\alpha = 109.47°$ (rhombohedral axes) or a triple hexagonal cell with $a_h = a_c\sqrt{2}$ and $c_h = a_c \frac{1}{2}\sqrt{3}$ (hexagonal axes).

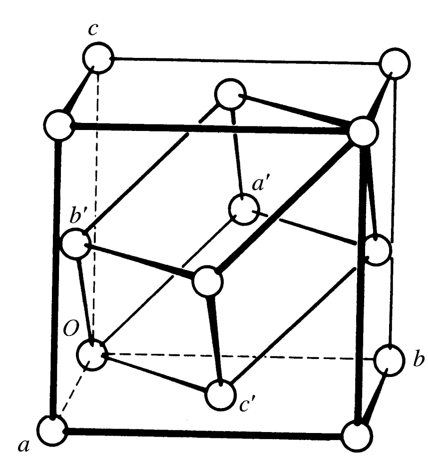


Fig. 5.1.3.4. Face-centred cell *F* with *a*, *b*, *c* and a corresponding primitive cell *P* with *a*′, *b*′, *c*′. Origin for both cells *O*. A cubic *F* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_r = a_c \frac{1}{2}\sqrt{2}$ and $\alpha = 60°$ (rhombohedral axes) or a triple hexagonal cell with $a_h = a_c \frac{1}{2}\sqrt{2}$ and $c_h = a_c\sqrt{3}$ (hexagonal axes).

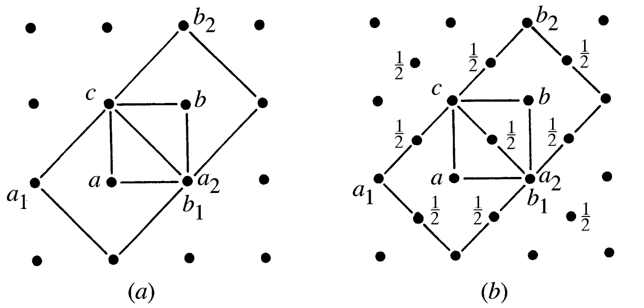


Fig. 5.1.3.5. Tetragonal lattices, projected along $[00\bar{1}]$. (a) Primitive cell P with a, b, c and the C-centred cells C_1 with a_1, b_1, c and C_2 with a_2, b_2, c. Origin for all three cells is the same. (b) Body-centred cell I with a, b, c and the F-centred cells F_1 with a_1, b_1, c and F_2 with a_2, b_2, c. Origin for all three cells is the same.

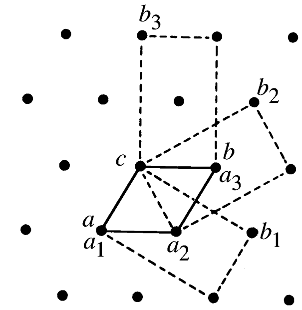


Fig. 5.1.3.7. Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three C-centred (orthohexagonal) cells a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. Origin for all cells is the same.

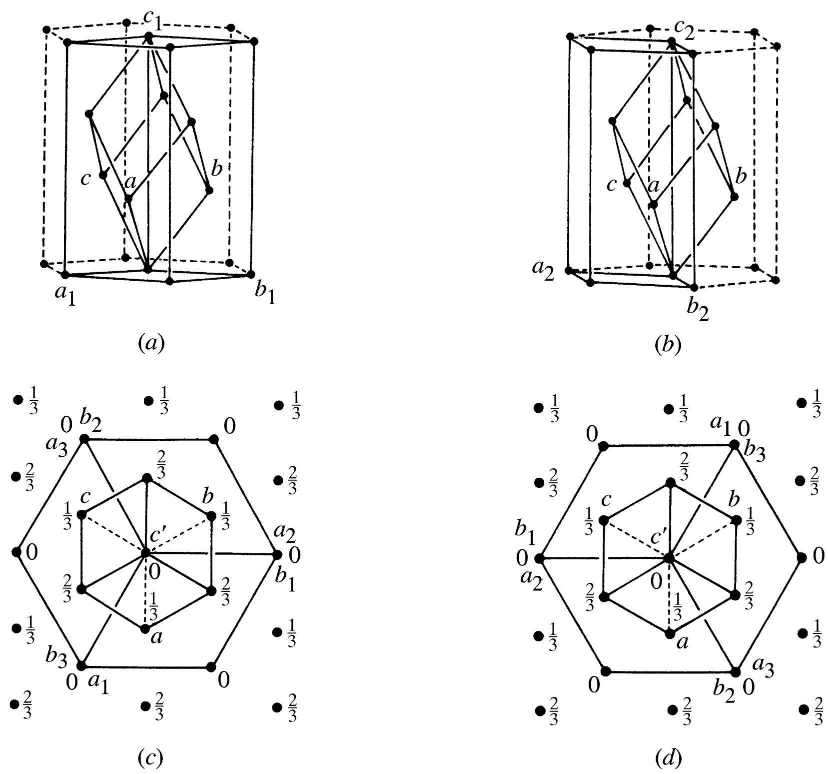


Fig. 5.1.3.6. Unit cells in the rhombohedral lattice: same origin for all cells. The basis of the rhombohedral cell is labelled a, b, c. Two settings of the triple hexagonal cell are possible with respect to a primitive rhombohedral cell: The *obverse setting* with the lattice points 0, 0, 0; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ 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 $h - k + l = 3n$. (a) Obverse setting of triple hexagonal cell a_1, b_1, c_1 in relation to the primitive rhombohedral cell a, b, c. (b) Reverse setting of triple hexagonal cell a_2, b_2, c_2 in relation to the primitive rhombohedral cell a, b, c. (c) Primitive rhombohedral cell (--- lower edges), a, b, c 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, b, c 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'.

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \mathbb{Q} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

$$= \begin{pmatrix} Q_{11}x + Q_{12}y + Q_{13}z + q_1 \\ Q_{21}x + Q_{22}y + Q_{23}z + q_2 \\ Q_{31}x + Q_{32}y + Q_{33}z + q_3 \\ 1 \end{pmatrix}.$$

The inverse of the augmented matrix $\mathbb{Q}$ is the augmented matrix $\mathbb{P}$ which contains the matrices $\boldsymbol{P}$ and $\boldsymbol{p}$, specifically,

$$\mathbb{P} = \mathbb{Q}^{-1} = \begin{pmatrix} \boldsymbol{P} & \boldsymbol{p} \\ \boldsymbol{o} & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{Q}^{-1} & -\boldsymbol{Q}^{-1}\boldsymbol{q} \\ \boldsymbol{o} & 1 \end{pmatrix}.$$

The advantage of the use of (4×4) matrices is that a sequence of affine transformations corresponds to the product of the correspond-

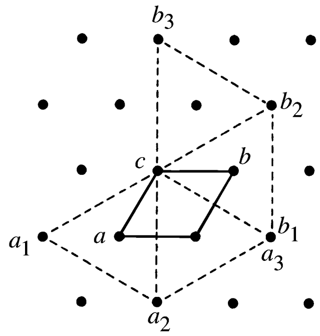
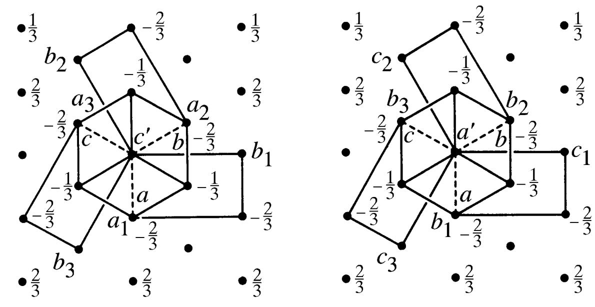
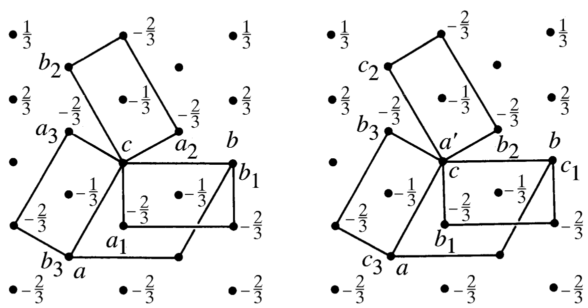


Fig. 5.1.3.8. Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three triple hexagonal cells H with a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. Origin for all cells is the same.



(*a*) (*b*)

Fig. 5.1.3.10. Rhombohedral lattice with primitive rhombohedral cell a, b, 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. 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. Origin for all four cells is the same.



(*a*) (*b*)

Fig. 5.1.3.9. 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. 5.1.3.6*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. 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. Origin for all four cells is the same.

ing matrices. However, the order of the factors in the product must be observed. If $\mathbb{Q}$ is the product of n transformation matrices $\mathbb{Q}_i$,

$$\mathbb{Q} = \mathbb{Q}_n \ldots \mathbb{Q}_2 \mathbb{Q}_1,$$

the sequence of the corresponding inverse matrices $\mathbb{P}_i$ is reversed in the product

$$\mathbb{P} = \mathbb{P}_1 \mathbb{P}_2 \ldots \mathbb{P}_n.$$

The following items are also affected by a transformation:

(i) The *metric matrix of direct lattice* $\boldsymbol{G}$ [more exactly: the matrix of geometrical coefficients (metric tensor)] is transformed by the matrix $\boldsymbol{P}$ as follows:

$$\boldsymbol{G}' = \boldsymbol{P}^t \boldsymbol{G} \boldsymbol{P}$$

with $\boldsymbol{P}^t$ the transposed matrix of $\boldsymbol{P}$, *i.e.* rows and columns of $\boldsymbol{P}$ are interchanged. Specifically,

$$\boldsymbol{G}' = \begin{pmatrix} \mathbf{a}'\cdot\mathbf{a}' & \mathbf{a}'\cdot\mathbf{b}' & \mathbf{a}'\cdot\mathbf{c}' \\ \mathbf{b}'\cdot\mathbf{a}' & \mathbf{b}'\cdot\mathbf{b}' & \mathbf{b}'\cdot\mathbf{c}' \\ \mathbf{c}'\cdot\mathbf{a}' & \mathbf{c}'\cdot\mathbf{b}' & \mathbf{c}'\cdot\mathbf{c}' \end{pmatrix}$$
$$= \begin{pmatrix} P_{11} & P_{21} & P_{31} \\ P_{12} & P_{22} & P_{32} \\ P_{13} & P_{23} & P_{33} \end{pmatrix} \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix}$$
$$\times \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}.$$

(ii) The *metric matrix of reciprocal lattice* $\boldsymbol{G}^*$ [more exactly: the matrix of geometrical coefficients (metric tensor)] is transformed by

$$\boldsymbol{G}^{*\prime} = \boldsymbol{Q} \boldsymbol{G}^* \boldsymbol{Q}^t.$$

Here, the transposed matrix $\boldsymbol{Q}^t$ is on the right-hand side of $\boldsymbol{G}^*$.

(iii) The *volume of the unit cell V* changes with the transformation. The volume of the new unit cell V' is obtained by

$$V' = \det(\boldsymbol{P})V = \begin{vmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{vmatrix} V$$

with $\det(\boldsymbol{P})$ the determinant of the matrix $\boldsymbol{P}$. The corresponding equation for the volume of the unit cell in reciprocal space V^* is

$$V^{*\prime} = \det(\boldsymbol{Q})V^*.$$

Matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ that frequently occur in crystallography are listed in Table 5.1.3.1.