

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.5.1.1 (continued)

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

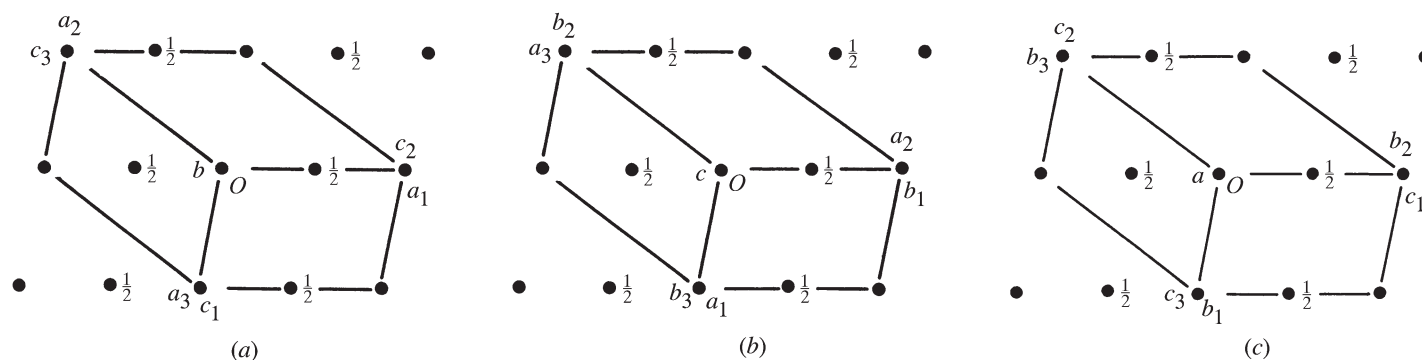


Figure 1.5.1.2

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 .

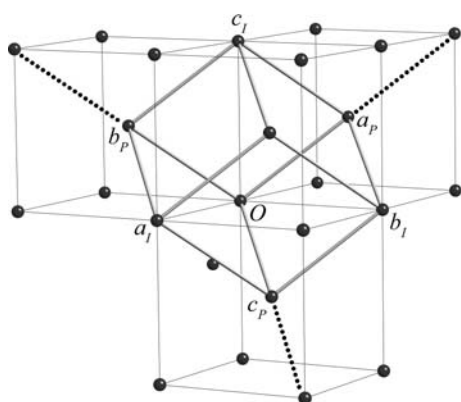


Figure 1.5.1.3

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 $a_{rh} = a_c \frac{1}{2} \sqrt{3}$ and $\alpha = 109.47^\circ$ (rhombohedral axes) or a triple hexagonal cell with $a_{hex} = a_c \sqrt{2}$ and $c_{hex} = a_c \frac{1}{2} \sqrt{3}$ (hexagonal axes).

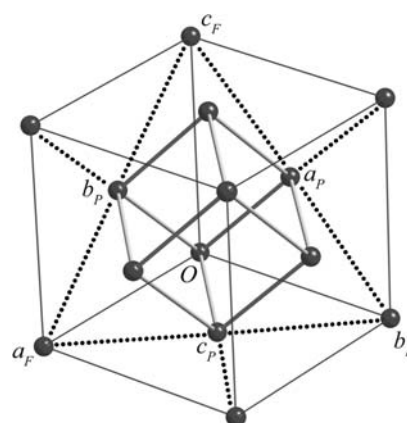


Figure 1.5.1.4

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 $a_{rh} = a_c \frac{1}{2} \sqrt{2}$ and $\alpha = 60^\circ$ (rhombohedral axes) or a triple hexagonal cell with $a_{hex} = a_c \frac{1}{2} \sqrt{2}$ and $c_{hex} = a_c \sqrt{3}$ (hexagonal axes).