

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 $b$ , 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 $c$ , 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 $c$ , 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 $c$ , 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)

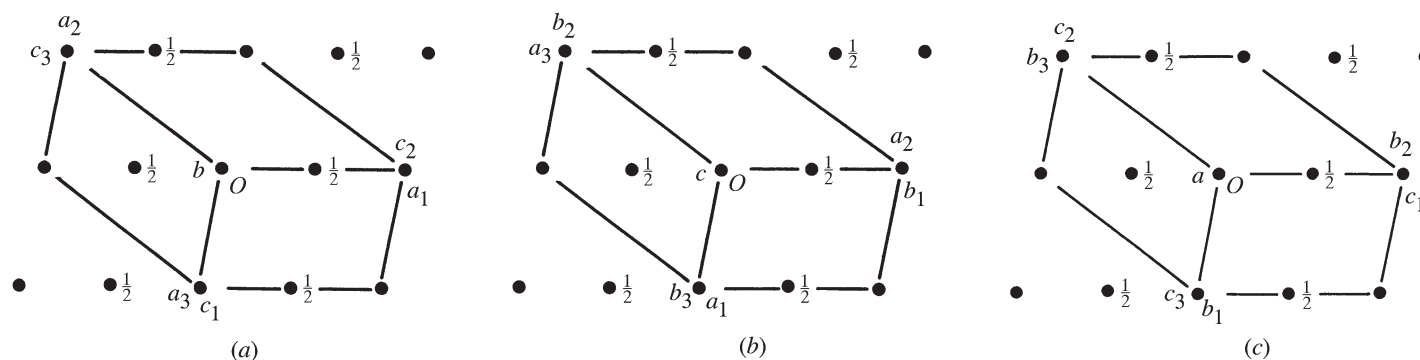


Figure 1.5.1.2

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  $a, b_3, c_3$ .

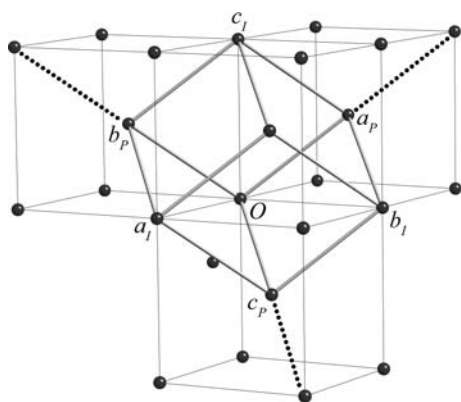


Figure 1.5.1.3

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).

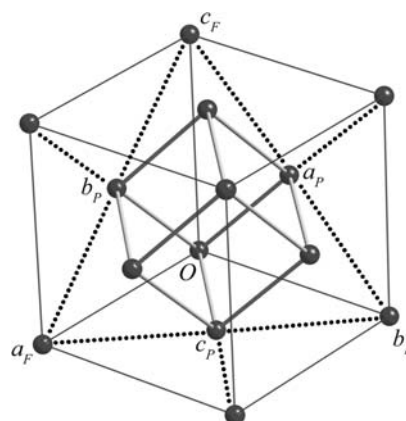


Figure 1.5.1.4

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).