

5. TRANSFORMATIONS IN CRYSTALLOGRAPHY

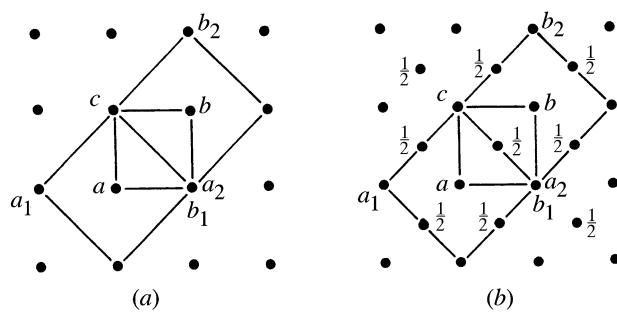
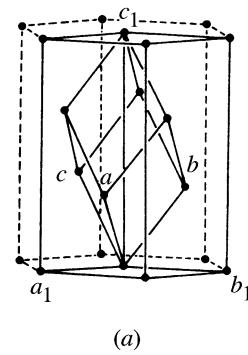
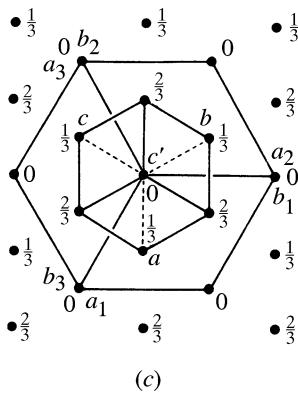


Fig. 5.1.3.5. Tetragonal lattices, projected along $[00\bar{1}]$. (a) Primitive cell P with a, b, c and the C -centred cells C_1 with a_1, b_1, c and C_2 with a_2, b_2, c . Origin for all three cells is the same. (b) Body-centred cell I with a, b, c and the F -centred cells F_1 with a_1, b_1, c and F_2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



(a)



(b)

(c)

(d)

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 \mathbf{P} and \mathbf{p} , specifically,

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

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