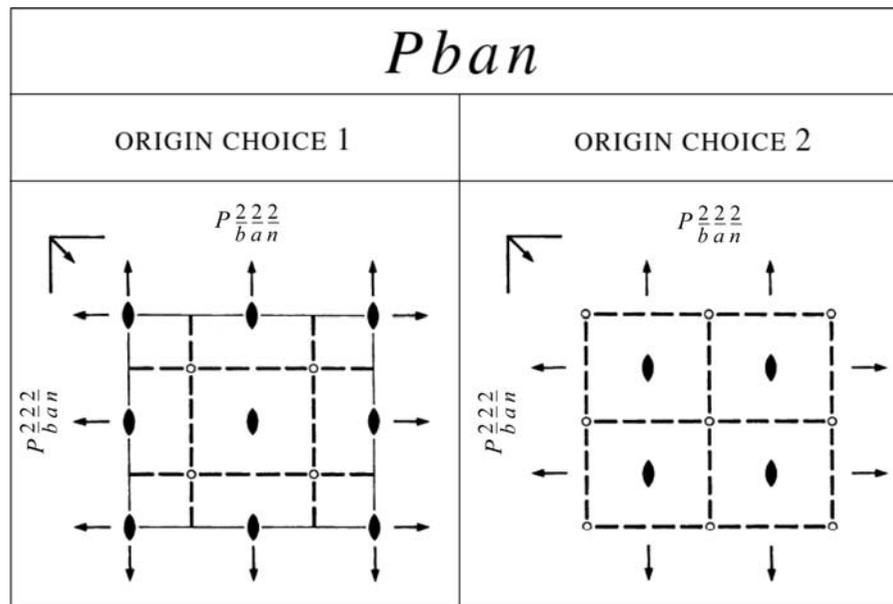


1. INTRODUCTION TO SPACE-GROUP SYMMETRY



**Figure 1.5.3.2** Two possible origin choices for the orthorhombic space group  $Pban$  (50). Origin choice 1 is on 222, whereas origin choice 2 is on  $\bar{1}$ .

hexagonal cell ( $|\mathbf{a}_{\text{hex}}| = |\mathbf{b}_{\text{hex}}|$ ;  $\mathbf{c}_{\text{hex}} \perp \mathbf{a}_{\text{hex}}, \mathbf{b}_{\text{hex}}$ ;  $\gamma = 120^\circ$ ) with a volume three times larger than that of the primitive rhombohedral cell. The second presentation is given with a primitive rhombohedral cell with  $a_{\text{rh}} = b_{\text{rh}} = c_{\text{rh}}$  and  $\alpha_{\text{rh}} = \beta_{\text{rh}} = \gamma_{\text{rh}}$ . The relation between the two types of cell is illustrated in Fig. 1.5.3.3 for the space group  $R3m$  (160). In the hexagonal cell, the coordinates of the special position with site symmetry  $3m$  are  $0, 0, z$ , whereas in the rhombohedral cell the same special position has coordinates  $x, x, x$ . If we refer to the transformations of the primitive rhombohedral cell cited in Table 1.5.1.1, we observe two different centring with three possible orientations  $R_1, R_2$  and  $R_3$  which are related by  $\pm 120^\circ$  to each other. The two kinds of centring, called *obverse* and *reverse*, are illustrated in Fig. 1.5.1.6. A rotation of  $180^\circ$  around the rhombohedral axis relates the obverse and reverse descriptions of the rhombohedral lattice. The obverse triple  $R$  cells have lattice points at  $0, 0, 0$ ;  $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ ;  $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ , whereas the reverse  $R$  cells have lattice points at  $0, 0, 0$ ;  $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$ ;  $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$ . The triple hexagonal cell  $R_1$  of the obverse setting (*i.e.*  $\mathbf{a}_{\text{hex}} = \mathbf{a}_{\text{rh}} - \mathbf{b}_{\text{rh}}$ ,  $\mathbf{b}_{\text{hex}} = \mathbf{b}_{\text{rh}} - \mathbf{c}_{\text{rh}}$ ,  $\mathbf{c}_{\text{hex}} = \mathbf{a}_{\text{rh}} + \mathbf{b}_{\text{rh}} + \mathbf{b}_{\text{rh}}$ ) has been used in the description of the rhombohedral space groups in this volume (*cf.* Table 1.5.1.1 and Fig. 1.5.3.3).

The hexagonal lattice can be referred to a centred rhombohedral cell, called the  $D$  cell (*cf.* Table 1.5.1.1). The centring points of this cell are  $0, 0, 0$ ,  $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$  and  $\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$ . However, the  $D$  cell is rarely used in crystallography.

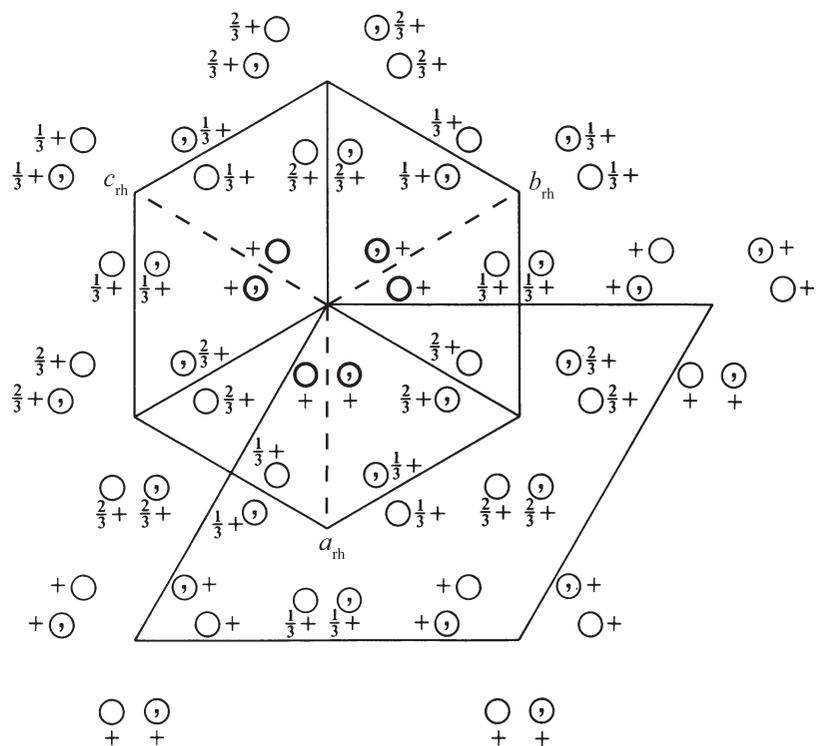
**1.5.3.2. Examples**

*1.5.3.2.1. Transformations between different settings of  $P2_1/c$*

In the space-group tables of this volume, the monoclinic space group  $P2_1/c$  (14) is described in six different settings: for each of the ‘unique axis  $b$ ’ and ‘unique axis  $c$ ’ settings there are three descriptions specified by different cell choices (*cf.* Section 2.1.3.15). The different settings are identified by the appropriate full Hermann–Mauguin symbols. The basis transfor-

mations ( $\mathbf{P}, \mathbf{p}$ ) between the different settings are completely specified by the linear part of the transformation, the  $3 \times 3$  matrix  $\mathbf{P}$  [*cf.* equation (1.5.1.4)], as all settings of  $P2_1/c$  refer to the same origin, *i.e.*  $\mathbf{p} = \mathbf{o}$ . The transformation matrices  $\mathbf{P}$  necessary for switching between the different descriptions of  $P2_1/c$  can either be read off directly or constructed from the transformation-matrix data listed in Table 1.5.1.1.

(A) Transformation from  $P12_1/c1$  (unique axis  $b$ , cell choice 1) to  $P112_1/a$  (unique axis  $c$ , cell choice 1). The change of the direction of the screw axis  $2_1$  indicates that the unique direction  $\mathbf{b}$



**Figure 1.5.3.3** General-position diagram of the space group  $R3m$  (160) showing the relation between the hexagonal and rhombohedral axes in the obverse setting:  $\mathbf{a}_{\text{rh}} = \frac{1}{3}(2\mathbf{a}_{\text{hex}} + \mathbf{b}_{\text{hex}} + \mathbf{c}_{\text{hex}})$ ,  $\mathbf{b}_{\text{rh}} = \frac{1}{3}(-\mathbf{a}_{\text{hex}} + \mathbf{b}_{\text{hex}} + \mathbf{c}_{\text{hex}})$ ,  $\mathbf{c}_{\text{rh}} = \frac{1}{3}(-\mathbf{a}_{\text{hex}} - 2\mathbf{b}_{\text{hex}} + \mathbf{c}_{\text{hex}})$ .