$$(\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1}) = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}_1 = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (1.5.3.1)$$

Step 2. Cell choice 1 invariant: transformation from unique axis c to unique axis b:

$$(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) = (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\boldsymbol{P}_2 = (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \quad (1.5.3.2)$$

The transformation matrix $\boldsymbol{P}$ for the change from $P112_1/b$ to $P12_1/c1$ is obtained by starting from equation (1.5.3.2) and replacing the expression for $\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1}$ with that from equation (1.5.3.1):

$$\begin{aligned}(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) &= (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\boldsymbol{P}_2 = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}_1\boldsymbol{P}_2 \\ &= (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\ &= (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.\end{aligned}$$

The inverse matrix $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ can be obtained either by inversion or by the product of the factors $\boldsymbol{Q}_1 = \boldsymbol{P}_1^{-1}$ and $\boldsymbol{Q}_2 = \boldsymbol{P}_2^{-1}$ but in reverse order:

$$\boldsymbol{Q} = (\boldsymbol{P}_1\boldsymbol{P}_2)^{-1} = \boldsymbol{P}_2^{-1}\boldsymbol{P}_1^{-1} = \boldsymbol{Q}_2\boldsymbol{Q}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ \bar{1} & 1 & 0 \end{pmatrix}.$$

The transformation matrix $\boldsymbol{P}$ determined above and its inverse $\boldsymbol{Q}$ permit the transformation of crystallographic data for the change from $P112_1/b$ to $P12_1/c1$.

1.5.3.2.2. *Transformation between the two origin-choice settings of* $I4_1/amd$

The zircon example of Section 1.5.1.1 illustrates how the atomic coordinates change under an origin-choice transformation. Here, the case of the two origin-choice descriptions of the same space group $I4_1/amd$ (141) will be used to demonstrate how the rest of the crystallographic quantities are affected by an origin shift.

The two descriptions of $I4_1/amd$ in the space-group tables of this volume are distinguished by the origin choices of the reference coordinate systems: the origin statement of the origin choice 1 setting indicates that its origin O_1 is taken at a point of $\bar{4}m2$ symmetry, which is located at $0, \frac{1}{4}, -\frac{1}{8}$ with respect to the origin O_2 of origin choice 2, taken at a centre ($2/m$). Conversely, the origin O_2 is taken at a centre ($2/m$) at $0, -\frac{1}{4}, \frac{1}{8}$ from the origin O_1. These origin descriptions in fact specify explicitly the origin-shift vector $\boldsymbol{p}$ necessary for the transformation between the two settings. For example, the shift vector listed for origin choice 2 expresses the origin O_2 with respect to O_1, *i.e.* the corresponding transformation matrix

$$(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{I}, \boldsymbol{p}) = (\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -\frac{1}{4} \\ \frac{1}{8} \end{pmatrix})$$

transforms the crystallographic data from the origin choice 1 setting to the origin choice 2 setting.

(i) *Transformation of point coordinates.* In accordance with the discussion of Section 1.5.1.1 [*cf.* equation (1.5.1.2)], the transformation of point coordinates $\boldsymbol{x}_1 = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$ of the origin choice 1 setting of $I4_1/amd$ to $\boldsymbol{x}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$ of the origin choice 2 setting is given by

$$\boldsymbol{x}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} = (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x}_1 = (\boldsymbol{I}, -\boldsymbol{p})\boldsymbol{x}_1 = \begin{pmatrix} x_1 \\ y_1 + \frac{1}{4} \\ z_1 - \frac{1}{8} \end{pmatrix}. \quad (1.5.3.3)$$

(ii) *Metric tensors and the data for the reflection conditions*. The metric tensors and the data for the reflection conditions are not affected by an origin shift as $\boldsymbol{P} = \boldsymbol{I}$, *cf.* equations (1.5.2.4) and (1.5.2.2).

(iii) *Transformation of the matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$ *of the symmetry operations*. The origin-shift transformation $(\boldsymbol{I}, \boldsymbol{p})$ relates the matrix–column pairs $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ of the symmetry operations of the origin choice 1 setting of $I4_1/amd$ to $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ of the origin choice 2 setting [*cf.* equation (1.5.2.11)]:

$$(\boldsymbol{W}_2, \boldsymbol{w}_2) = (\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}_1, \boldsymbol{w}_1)(\boldsymbol{I}, \boldsymbol{p}) = (\boldsymbol{W}_1, \boldsymbol{w}_1 + [\boldsymbol{W}_1 - \boldsymbol{I}]\boldsymbol{p}). \quad (1.5.3.4)$$

The rotation part of the symmetry operation is not affected by the origin shift, but the translation part is affected, *i.e.* $\boldsymbol{W}_2 = \boldsymbol{W}_1$ and $\boldsymbol{w}_2 = \boldsymbol{w}_1 + [\boldsymbol{W}_1 - \boldsymbol{I}]\boldsymbol{p}$. For example, the translation and unit element generators of $I4_1/amd$ are not changed under the origin-shift transformation, as $\boldsymbol{W}_1 = \boldsymbol{I}$. The first non-translation generator given by the coordinate triplet $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ and represented by the matrix

$$(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}) \text{ transforms to } (\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} \frac{1}{4} \\ \frac{3}{4} \\ \frac{1}{4} \end{pmatrix}),$$

which corresponds to the coordinate triplet $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$.

The second non-translation generator $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$, represented by the matrix

$$(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}) \text{ transforms to } (\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}),$$

which under the normalization $0 \le w_i < 1$ is written as the coordinate triplet $\bar{x}, \bar{y}, \bar{z}$. The coordinate triplets of the transformed symmetry operations are the entries of the corresponding generators of the origin choice 2 setting of $I4_1/amd$ (*cf.* the space-group tables of $I4_1/amd$ in Chapter 2.3).

references