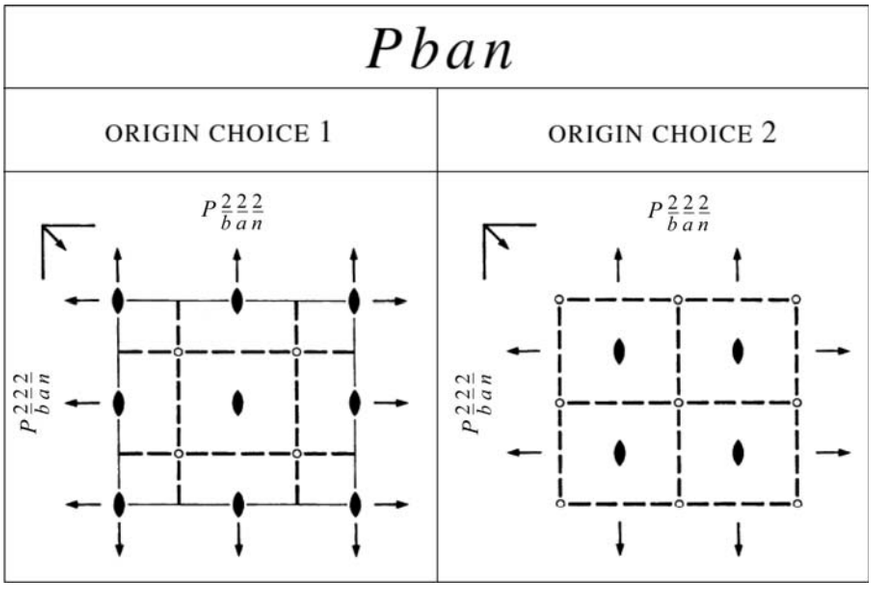

Figure 1.5.3.2
Two possible origin choices for the orthorhombic space group *Pban* (50). Origin choice 1 is on 222, whereas origin choice 2 is on $\bar{1}$.

hexagonal cell ($|\mathbf{a}_{hex}| = |\mathbf{b}_{hex}|$; $\mathbf{c}_{hex} \perp \mathbf{a}_{hex}, \mathbf{b}_{hex}$; $\gamma = 120°$) with a volume three times larger than that of the primitive rhombohedral cell. The second presentation is given with a primitive rhombohedral cell with $a_{rh} = b_{rh} = c_{rh}$ and $\alpha_{rh} = \beta_{rh} = \gamma_{rh}$. The relation between the two types of cell is illustrated in Fig. 1.5.3.3 for the space group *R*3*m* (160). In the hexagonal cell, the coordinates of the special position with site symmetry 3*m* 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 centrings with three possible orientations R_1, R_2 and R_3 which are related by ±120° to each other. The two kinds of centrings, called *obverse* and *reverse*, are illustrated in Fig. 1.5.1.6. A rotation of 180° 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.* $\mathbf{a}_{hex} = \mathbf{a}_{rh} - \mathbf{b}_{rh}$, $\mathbf{b}_{hex} = \mathbf{b}_{rh} - \mathbf{c}_{rh}$, $\mathbf{c}_{hex} = \mathbf{a}_{rh} + \mathbf{b}_{rh} + \mathbf{b}_{rh}$) 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 transformations $(\boldsymbol{P}, \boldsymbol{p})$ between the different settings are completely specified by the linear part of the transformation, the 3 × 3 matrix $\boldsymbol{P}$ [*cf.* equation (1.5.1.4)], as all settings of $P2_1/c$ refer to the same origin, *i.e.* $\boldsymbol{p} = \boldsymbol{o}$. The transformation matrices $\boldsymbol{P}$ 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 **b**

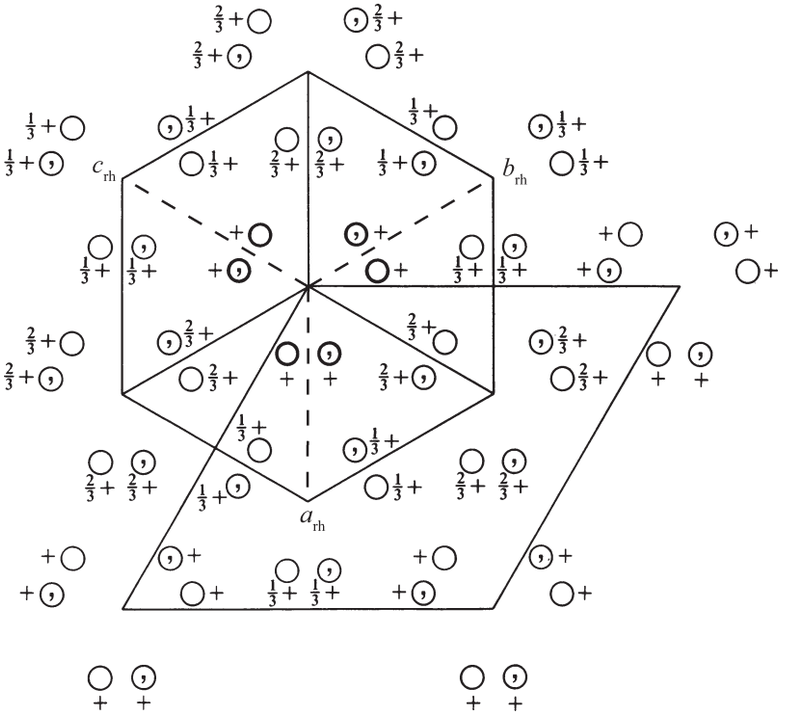

Figure 1.5.3.3
General-position diagram of the space group *R*3*m* (160) showing the relation between the hexagonal and rhombohedral axes in the obverse setting: $\mathbf{a}_{rh} = \frac{1}{3}(2\mathbf{a}_{hex} + \mathbf{b}_{hex} + \mathbf{c}_{hex})$, $\mathbf{b}_{rh} = \frac{1}{3}(-\mathbf{a}_{hex}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

Table 1.5.3.1
Transformation of reflection-condition data for $P12_1/c1$ to $P112_1/a$

	$P12_1/c1$ $h_bk_bl_b$	$P112_1/a$ $h_ck_cl_c$
General conditions	$h0l$: $l = 2n$ $0k0$: $k = 2n$ $00l$: $l = 2n$	$hk0$: $h = 2n$ $00l$: $l = 2n$ $h00$: $h = 2n$
Special conditions for the inversion centres	hkl: $k + l = 2n$	hkl: $h + l = 2n$

transforms to the unique direction **c**, while the glide vector along **c** transforms to a glide vector along **a**. These changes are reflected in the transformation matrix $\boldsymbol{P}$ between the basis $\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b$ of $P12_1/c1$ and $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ of $P112_1/a$, which can be read directly from Table 1.5.1.1:

$$(\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c) = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\boldsymbol{P} = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

(i) *Transformation of point coordinates*. From $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x}$, *cf.* equation (1.5.1.5), it follows that

$$\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} x_b \\ y_b \\ z_b \end{pmatrix} = \begin{pmatrix} z_b \\ x_b \\ y_b \end{pmatrix}.$$

For example, the representative coordinate triplets of the special Wyckoff position $2d\ \bar{1}$ of $P12_1/c1$ transform exactly to the representative coordinate triplets of the special Wyckoff position $2d\ \bar{1}$ of $P112_1/a$: $\begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ transform to $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$.

(ii) *Transformation of the indices in the 'Reflection conditions' block*. Under a coordinate transformation specified by a matrix $\boldsymbol{P}$, the indices of the reflection conditions (Miller indices) transform according to $(h'k'l') = (hkl)\boldsymbol{P}$, *cf.* equation (1.5.2.2). The transformation under

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

of the set of general or special reflection conditions $h_bk_bl_b$ for $P12_1/c1$ should result in the set of general or special reflection conditions $h_ck_cl_c$ of $P112_1/a$:

$$(h_ck_cl_c) = (h_bk_bl_b)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (l_bh_bk_b),$$

i.e. $h_c = l_b, k_c = h_b, l_c = k_b$ (see Table 1.5.3.1).

(iii) *Transformation of the matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$ *of the symmetry operations*. The matrices of the representatives of the symmetry operations of $P12_1/c1$ can be constructed from the coordinate triplets listed in the general-position block of the group:

(1) x, y, z (2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$

Their transformation is more conveniently performed using the augmented-matrix formalism. According to equation (1.5.2.17), the matrices $\mathbb{W}_c$ of the symmetry operations of $P112_1/a$ are related to the matrices $\mathbb{W}_b$ of $P12_1/c1$ by the equation $\mathbb{W}_c = \mathbb{Q}\mathbb{W}_b\mathbb{P}$, where

$$\mathbb{P} = \left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \quad \text{and} \quad \mathbb{Q} = \left(\begin{array}{ccc|c} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

The unit matrix representing the identity operation (1) is invariant under any basis transformation, *i.e.* x, y, z transforms to x, y, z. Similarly, the matrix of inversion $\bar{1}$ (3) (the linear part of which is a multiple of the unit matrix) is also invariant under any basis transformation, *i.e.* $\bar{x}, \bar{y}, \bar{z}$ transforms to $\bar{x}, \bar{y}, \bar{z}$. The symmetry operation (2) $\bar{x},\ y + \frac{1}{2},\ \bar{z} + \frac{1}{2}$, represented by the matrix

$$\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

transforms to

$$\left(\begin{array}{ccc|c} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)\left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$
$$= \left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

which corresponds to $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$.

Finally, the symmetry operation (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ represented by the matrix

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \text{ transforms to } \left(\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

corresponding to the coordinate triplet $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ [the matrices of (4) and its transformed are those of (2) and its transformed, multiplied by $\bar{1}$].

The coordinate triplets of the transformed symmetry operations correspond to the entries of the general-position block of $P112_1/a$ (*cf.* the space-group tables of $P2_1/c$ in Chapter 2.3).

(*B*) *Transformation from* $P112_1/b$ *(unique axis c, cell choice 3) to* $P12_1/c1$ *(unique axis b, cell choice 1)*: $(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}$. A transformation matrix from $P112_1/b$ directly to $P12_1/c1$ is not found in Table 1.5.1.1, but it can be constructed in two steps from transformation matrices that are listed there. For example:

Step 1. Unique axis *c* fixed: transformation from 'cell choice 3' to 'cell choice 1':

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

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

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

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

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

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

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

which under the normalization $0 \leq w_i < 1$ 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).