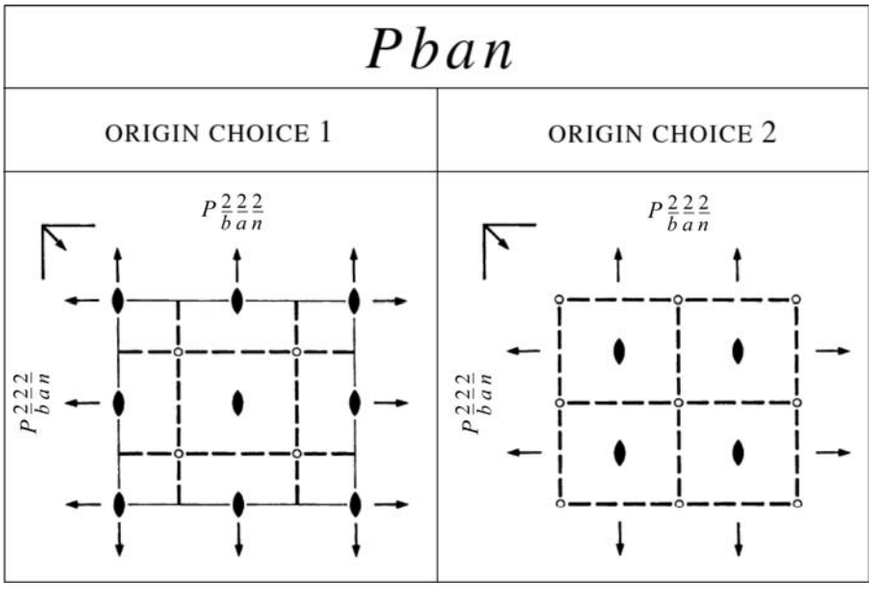

Figure 1.5.3.2
Two possible origin choices for the orthorhombic space group *Pban* (50). Origin choice 1 is on 222, whereas origin choice 2 is on $\bar{1}$.

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**

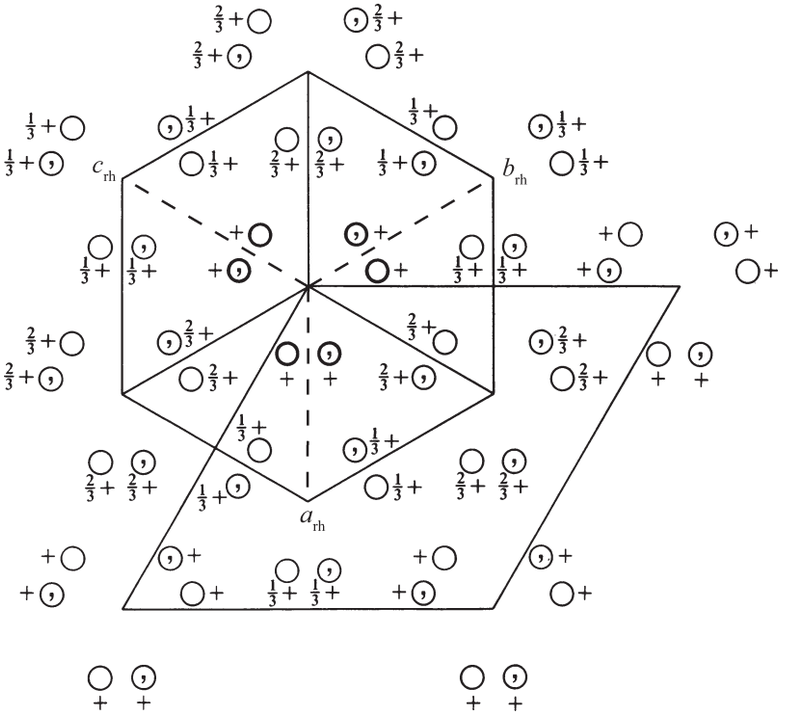

Figure 1.5.3.3
General-position diagram of the space group *R*3*m* (160) showing the relation between the hexagonal and rhombohedral axes in the obverse setting: $\mathbf{a}_{rh} = \frac{1}{3}(2\mathbf{a}_{hex} + \mathbf{b}_{hex} + \mathbf{c}_{hex})$, $\mathbf{b}_{rh} = \frac{1}{3}(-\mathbf{a}_{hex}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

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).