

## 1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

mined lattice parameters of the low-symmetry phase [ $a_{\text{hex}} = 4.164(2) \text{ \AA}$ ,  $c_{\text{hex}} = 10.69(4) \text{ \AA}$  (Chattopadhyay *et al.*, 1987)] determines the lattice deformation accompanying the displacive phase transition, which basically consists of expanding the cubic unit cell along the [111] direction. (In fact, the elongation along [111] is accompanied by a contraction in the  $ab$  plane that leads to an overall volume reduction of about 1.3%.)

Owing to the polar character of  $R3m$ , the symmetry conditions following from the group–subgroup relation  $Fm\bar{3}m > R3m$  [cf. equation (1.5.2.11)] are not sufficient to determine the origin shift of the transformation between the high- and the low-symmetry space groups. The origin shift of  $\mathbf{p} = (-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4})$  in this specific case is chosen in such a way that the relative displacements of Ge and Te are equal in size but in opposite direction along [111].

The inverse transformation matrix–column pair  $(\mathbf{Q}, \mathbf{q}) = (\mathbf{P}, \mathbf{p})^{-1} = (\mathbf{P}^{-1}, -\mathbf{P}^{-1}\mathbf{p})$  is necessary for the calculation of the atomic coordinates of the reference description  $X'_c$ . Given the matrix  $\mathbf{P}$ , its inverse  $\mathbf{P}^{-1}$  can be calculated either directly (*i.e.* applying the algebraic procedure for inversion of a matrix) or using the inverse matrices  $\mathbf{Q}_1 = \mathbf{P}_1^{-1}$  and  $\mathbf{Q}_2 = \mathbf{P}_2^{-1}$  listed in Table 1.5.1.1:

$$\begin{aligned}
 \mathbf{Q} = \mathbf{P}^{-1} &= (\mathbf{P}_1\mathbf{P}_2)^{-1} = \mathbf{P}_2^{-1}\mathbf{P}_1^{-1} \\
 &= \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix} = \begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}.
 \end{aligned} \quad (1.5.2.22)$$

(Note the change in the order of multiplication of the matrices  $\mathbf{P}_1^{-1}$  and  $\mathbf{P}_2^{-1}$  in  $\mathbf{Q}$ .) The corresponding origin shift  $\mathbf{q}$  is given by

$$\mathbf{q} = -\mathbf{P}^{-1}\mathbf{p} = -\begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} -\frac{1}{4} \\ -\frac{1}{4} \\ -\frac{1}{4} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}. \quad (1.5.2.23)$$

The atomic positions of the reference description become

$$\begin{pmatrix} x'_c \\ y'_c \\ z'_c \end{pmatrix} = \begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}.$$

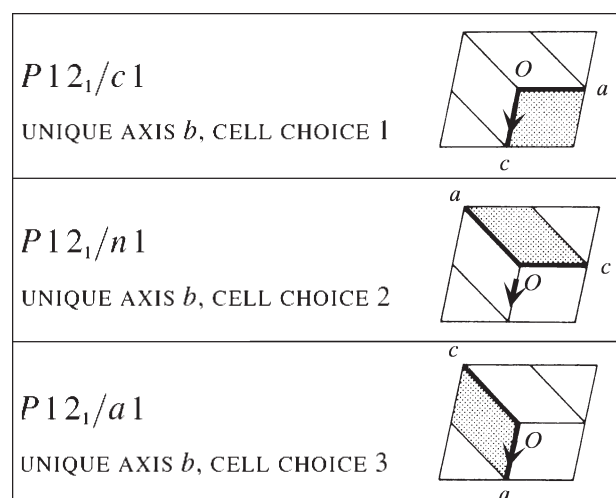
The coordinates of the representative Ge atom occupying position  $4a \ 0, 0, 0$  in  $Fm\bar{3}m$  are transformed to  $0, 0, \frac{1}{4}$ , while those of Te are transformed from  $4b \ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$  in  $Fm\bar{3}m$  to  $0, 0, \frac{3}{4}$ . The comparison of these values with the experimentally determined atomic coordinates of Ge  $0, 0, 0.2376$  and Te  $0, 0, 0.7624$  reveals the corresponding atomic displacements associated with the displacive phase transition. The low-symmetry phase is a result of relative atomic displacements of the Ge and Te atoms along the polar (rhombohedral) [111] direction, giving rise to non-zero polarization along the same direction, *i.e.* the phase transition is a *paraelectric-to-ferroelectric* one.

### 1.5.3. Transformations between different space-group descriptions

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#### 1.5.3.1. Space groups with more than one description in this volume

In the description of the space-group symbols presented in Section 1.4.1, we have already seen that in the conventional,



**Figure 1.5.3.1**

Three possible cell choices for the monoclinic space group  $P2_1/c$  (14) with unique axis  $b$ . Note the corresponding changes in the full Hermann–Mauguin symbols. The glide vector is indicated by an arrow.

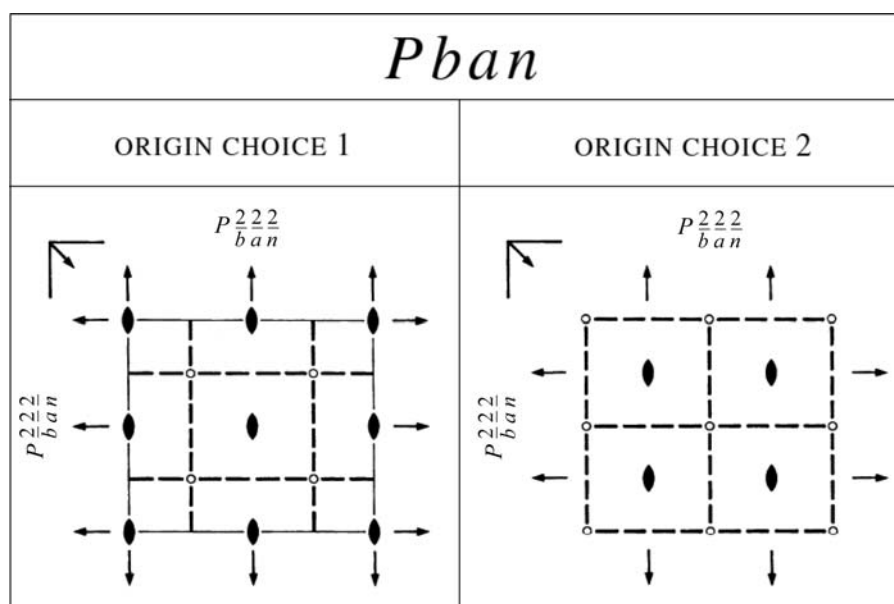
*unique axis b* description of monoclinic space groups, the unique symmetry direction is chosen as  $\mathbf{b}$ ; it is normal to  $\mathbf{c}$  and  $\mathbf{a}$ , which form the angle  $\beta$ . However, it is often the case that this standard direction is not the most appropriate choice and that another choice would be more convenient. An example of this would be when following a phase transition from an orthorhombic parent phase to a monoclinic phase. Here, it would often be preferable to keep the same orientation of the axes even if the resulting monoclinic setting is not standard.

In some of the space groups, and especially in the monoclinic ones, the space-group tables of Chapter 2.3 provide a selection of possible alternative settings. For example, in space group  $P2_1/c$ , two possible orientations of the unit-cell axes are provided, namely with unique axis  $b$  and  $c$ . This is reflected in the corresponding full Hermann–Mauguin symbols by the explicit specification of the unique-axis position (dummy indices ‘1’ indicate ‘empty’ symmetry directions), and by the corresponding change in the direction of the glide plane:  $P12_1/c1$  or  $P112_1/a$  (cf. Section 1.4.1 for a detailed treatment of Hermann–Mauguin symbols of space groups).

It is not just the unique monoclinic axis that can be varied: the choice of the other axes can vary as well. There are cases where the selection of the conventional setting leads to an inconvenient monoclinic angle that deviates greatly from  $90^\circ$ . If another cell choice minimizes the deviation from  $90^\circ$ , it is preferred. Fig. 1.5.3.1 illustrates three cell choices for the monoclinic axis  $b$  setting of  $P2_1/c$ .

In centrosymmetric space groups the origin of the unit cell is located at an inversion centre (‘origin choice 2’). If, however, another point has higher site symmetry  $\mathcal{S}$ , a second diagram is displayed with the origin at a point with site symmetry  $\mathcal{S}$  (‘origin choice 1’). Fig. 1.5.3.2 illustrates the space group  $Pban$  with two possible origins. The origin of the first choice is located on a point with site symmetry  $222$ , whereas the origin for the second choice is located on an inversion centre. Among the 230 space groups, this volume lists 24 centrosymmetric space groups with an additional alternative origin.

Finally, the seven rhombohedral space-group types (*i.e.* space groups with a rhombohedral lattice) also have alternative descriptions included in the space-group tables of this volume. The rhombohedral lattice is first presented with an  $R$ -centred


**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.

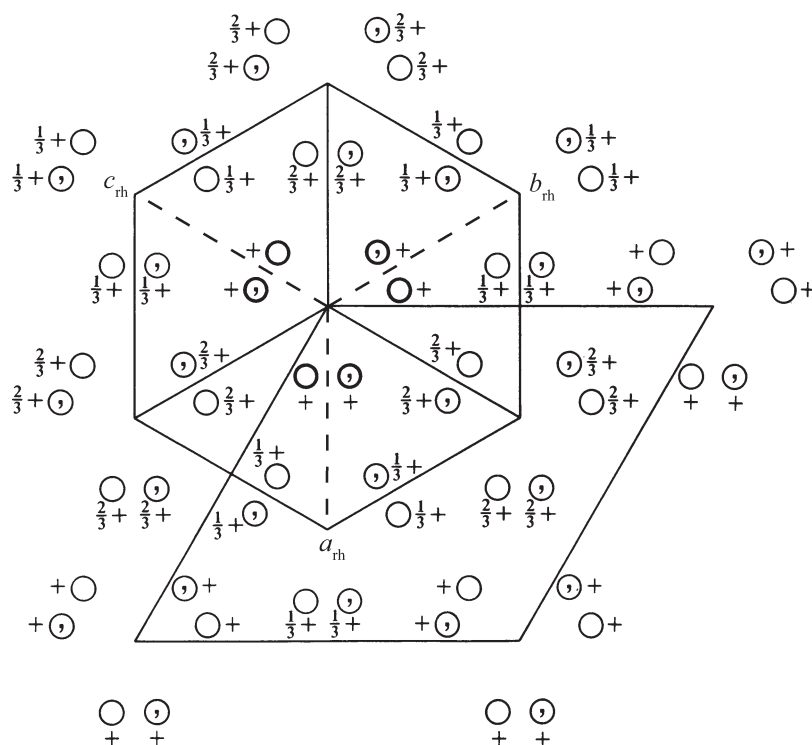
### 1.5.3.2. Examples

#### 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:  $\mathbf{a}_{\text{rh}} = \frac{1}{3}(2\mathbf{a}_{\text{hex}} + \mathbf{b}_{\text{hex}} + \mathbf{c}_{\text{hex}})$ ,  $\mathbf{b}_{\text{rh}} = \frac{1}{3}(-\mathbf{a}_{\text{hex}} + \mathbf{b}_{\text{hex}} + \mathbf{c}_{\text{hex}})$ ,  $\mathbf{c}_{\text{rh}} = \frac{1}{3}(-\mathbf{a}_{\text{hex}} - 2\mathbf{b}_{\text{hex}} + \mathbf{c}_{\text{hex}})$ .

## 1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

**Table 1.5.3.1**

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

	$P12_1/c1$ $h_b k_b l_b$	$P112_1/a$ $h_c k_c l_c$
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  $\mathbf{c}$ , while the glide vector along  $\mathbf{c}$  transforms to a glide vector along  $\mathbf{a}$ . These changes are reflected in the transformation matrix  $\mathbf{P}$  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:

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

- (i) *Transformation of point coordinates.* From  $\mathbf{x}' = \mathbf{P}^{-1}\mathbf{x}$ , 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  $\mathbf{P}$ , the indices of the reflection conditions (Miller indices) transform according to  $(h'k'l') = (hkl)\mathbf{P}$ , cf. equation (1.5.2.2). The transformation under

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

of the set of general or special reflection conditions  $h_b k_b l_b$  for  $P12_1/c1$  should result in the set of general or special reflection conditions  $h_c k_c l_c$  of  $P112_1/a$ :

$$(h_c k_c l_c) = (h_b k_b l_b) \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (l_b h_b k_b),$$

*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  $(\mathbf{W}, \mathbf{w})$  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:

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

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  $\mathbb{W}_c = \mathbb{Q}\mathbb{W}_b\mathbf{P}$ , where

$$\mathbf{P} = \begin{pmatrix} 0 & 1 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix} \quad \text{and} \quad \mathbb{Q} = \begin{pmatrix} 0 & 0 & 1 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & 0 \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix}.$$

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

$$\begin{pmatrix} \bar{1} & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & \frac{1}{2} \\ 0 & 0 & \bar{1} & | & \frac{1}{2} \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix}$$

transforms to

$$\begin{pmatrix} 0 & 0 & 1 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & 0 \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix} \begin{pmatrix} \bar{1} & 0 & 0 & | & 0 \\ 0 & 1 & 0 & | & \frac{1}{2} \\ 0 & 0 & \bar{1} & | & \frac{1}{2} \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & | & 0 \\ 0 & 0 & 1 & | & 0 \\ 1 & 0 & 0 & | & 0 \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix} \\ = \begin{pmatrix} \bar{1} & 0 & 0 & | & \frac{1}{2} \\ 0 & \bar{1} & 0 & | & 0 \\ 0 & 0 & 1 & | & \frac{1}{2} \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix},$$

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

$$\begin{pmatrix} 1 & 0 & 0 & | & 0 \\ 0 & \bar{1} & 0 & | & \frac{1}{2} \\ 0 & 0 & 1 & | & \frac{1}{2} \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix} \quad \text{transforms to} \quad \begin{pmatrix} 1 & 0 & 0 & | & \frac{1}{2} \\ 0 & 1 & 0 & | & 0 \\ 0 & 0 & \bar{1} & | & \frac{1}{2} \\ \hline 0 & 0 & 0 & | & 1 \end{pmatrix},$$

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):*  $(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\mathbf{P}$ . 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':

## 1. INTRODUCTION TO SPACE-GROUP SYMMETRY

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

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

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

The transformation matrix  $\mathbf{P}$  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):

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

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

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

The transformation matrix  $\mathbf{P}$  determined above and its inverse  $\mathbf{Q}$  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  $4m2$  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  $\mathbf{p}$  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

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

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  $\mathbf{x}_1 = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$  of the

origin choice 1 setting of  $I4_1/amd$  to  $\mathbf{x}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$  of the origin choice 2 setting is given by

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

(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  $\mathbf{P} = \mathbf{I}$ , *cf.* equations (1.5.2.4) and (1.5.2.2).

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

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

The rotation part of the symmetry operation is not affected by the origin shift, but the translation part is affected, *i.e.*  $\mathbf{W}_2 = \mathbf{W}_1$  and  $\mathbf{w}_2 = \mathbf{w}_1 + [\mathbf{W}_1 - \mathbf{I}]\mathbf{p}$ . For example, the translation and unit element generators of  $I4_1/amd$  are not changed under the origin-shift transformation, as  $\mathbf{W}_1 = \mathbf{I}$ . 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).