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:

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

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':