

## 1.5. TRANSFORMATIONS OF COORDINATE SYSTEMS

$$\begin{aligned} \begin{pmatrix} x_P \\ y_P \\ z_P \end{pmatrix} &= \mathbf{P}^{-1} \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} \\ &= \begin{pmatrix} -x_F + y_F + z_F \\ x_F - y_F + z_F \\ x_F + y_F - z_F \end{pmatrix}. \end{aligned}$$

For example, the coordinates  $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_F$  of the end point of  $\mathbf{a}_F$  with respect to the conventional basis become  $\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}_P$  in the primitive basis, the centring point  $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}_F$  of the  $\mathbf{a}_F, \mathbf{b}_F$  plane becomes the end point  $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_P$  of  $\mathbf{c}_P$  etc.

## 1.5.1.3. General change of coordinate system

A general change of the coordinate system involves both an origin shift and a change of the basis. Such a transformation of the coordinate system is described by the matrix-column pair  $(\mathbf{P}, \mathbf{p})$ , where the  $(3 \times 3)$  matrix  $\mathbf{P}$  relates the new basis  $\mathbf{a}', \mathbf{b}', \mathbf{c}'$  to the old one  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  according to equation (1.5.1.4). The origin shift is described by the *shift vector*  $\mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}$ . The coordinates of the new origin  $O'$  with respect to the old coordinate system  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  are given by the  $(3 \times 1)$  column  $\mathbf{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$ .

The general coordinate transformation can be performed in two consecutive steps. Because the origin shift  $\mathbf{p}$  refers to the old basis  $\mathbf{a}, \mathbf{b}, \mathbf{c}$ , it has to be applied first (as described in Section 1.5.1.1), followed by the change of the basis (cf. Section 1.5.1.2):

$$\mathbf{x}' = (\mathbf{P}, \mathbf{o})^{-1}(\mathbf{I}, \mathbf{p})^{-1}\mathbf{x} = ((\mathbf{I}, \mathbf{p})(\mathbf{P}, \mathbf{o}))^{-1}\mathbf{x} = (\mathbf{P}, \mathbf{p})^{-1}\mathbf{x}. \quad (1.5.1.6)$$

Here,  $\mathbf{I}$  is the three-dimensional unit matrix and  $\mathbf{o}$  is the  $(3 \times 1)$  column matrix containing only zeros as coefficients.

The formulae for the change of the *point coordinates* from  $\mathbf{x}$  to  $\mathbf{x}'$  uses  $(\mathbf{Q}, \mathbf{q}) = (\mathbf{P}, \mathbf{p})^{-1} = (\mathbf{P}^{-1}, -\mathbf{P}^{-1}\mathbf{p})$ , i.e.

$$\begin{aligned} \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix} &= \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} \\ &\text{with } \mathbf{Q} = \mathbf{P}^{-1} \text{ and } \mathbf{q} = -\mathbf{P}^{-1}\mathbf{p}, \\ &\text{thus } \mathbf{x}' = \mathbf{P}^{-1}\mathbf{x} - \mathbf{P}^{-1}\mathbf{p} = \mathbf{P}^{-1}(\mathbf{x} - \mathbf{p}). \end{aligned} \quad (1.5.1.7)$$

The effect of a general change of the coordinate system  $(\mathbf{P}, \mathbf{p})$  on the coefficients of a vector  $\mathbf{r}$  is reduced to the linear transformation described by  $\mathbf{P}$ , as the vector coefficients are not affected by the origin shift [cf. equation (1.5.1.3)].

Hereafter, the data for the matrix-column pair

$$(\mathbf{P}, \mathbf{p}) = \left( \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}, \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \right)$$

are often written in the following concise form:

$$\begin{aligned} P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \quad P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \quad P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}; \\ p_1, p_2, p_3. \end{aligned} \quad (1.5.1.8)$$

The concise notation of the transformation matrices is widely used in the tables of maximal subgroups of space groups in *International Tables for Crystallography* Volume A1 (2010), where  $(\mathbf{P}, \mathbf{p})$  describes the relation between the conventional bases of a group and its maximal subgroups. For example, the expression  $(\mathbf{P}, \mathbf{p}) = (\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}; 0, 0, \frac{1}{2})$  (cf. the table of maximal subgroups of  $P42m$ , No. 111, in Volume A1) stands for

$$\mathbf{P} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \text{ and } \mathbf{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}.$$

Note that the matrix elements of  $\mathbf{P}$  in equation (1.5.1.8) are read by *columns* since they act on the *row* matrices of basis vectors, and not by *rows*, as in the shorthand notation of symmetry operations which apply to *column* matrices of coordinates (cf. Section 1.2.2.1).

## 1.5.2. Transformations of crystallographic quantities under coordinate transformations

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## 1.5.2.1. Covariant and contravariant quantities

If the *direct* or *crystal* basis is transformed by the transformation matrix  $\mathbf{P}$ :  $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\mathbf{P}$ , the corresponding basis vectors of the *reciprocal* (or *dual*) basis transform as (cf. Section 1.3.2.5)

$$\begin{pmatrix} \mathbf{a}^{*'} \\ \mathbf{b}^{*'} \\ \mathbf{c}^{*'} \end{pmatrix} = \mathbf{Q} \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix} \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}, \quad (1.5.2.1)$$

where the notation  $\mathbf{Q} = \mathbf{P}^{-1}$  is applied (cf. Section 1.5.1.2).

The quantities that transform in the same way as the basis vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  are called *covariant* with respect to the basis  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  and *contravariant* with respect to the reciprocal basis  $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$ .

Such quantities are the *Miller indices*  $(hkl)$  of a plane (or a set of planes) in direct space and the vector coefficients  $(h, k, l)$  of the vector perpendicular to those planes, referred to the reciprocal basis  $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$ :

$$(h', k', l') = (h, k, l)\mathbf{P}. \quad (1.5.2.2)$$

Quantities like the vector coefficients of any vector  $\mathbf{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}$  in direct space (or the *indices of a direction* in direct space) are covariant with respect to the basis vectors  $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$  and contravariant with respect to  $\mathbf{a}, \mathbf{b}, \mathbf{c}$ :

$$\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = \mathbf{Q} \begin{pmatrix} u \\ v \\ w \end{pmatrix}. \quad (1.5.2.3)$$