International Tables for Crystallography (2016). Vol. A, Section 1.5.2.1, p. 83.

$$\begin{pmatrix} x_P \\ y_P \\ z_P \end{pmatrix} = \boldsymbol{P}^{-1}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}$$

$$= \begin{pmatrix} -x_F + y_F + z_F \\ x_F - y_F + z_F \\ x_F + y_F - z_F \end{pmatrix}.$$

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.*

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 $(\boldsymbol{P}, \boldsymbol{p})$ describes the relation between the conventional bases of a group and its maximal subgroups. For example, the expression $(\boldsymbol{P}, \boldsymbol{p}) = (\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}; 0, 0, \frac{1}{2})$ (*cf.* the table of maximal subgroups of $P\bar{4}2m$, No. 111, in Volume A1) stands for

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

Note that the matrix elements of $\boldsymbol{P}$ 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).

1.5.1.3. 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 $(\boldsymbol{P}, \boldsymbol{p})$, where the (3×3) matrix $\boldsymbol{P}$ 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 (3×1) column $\boldsymbol{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$.

The general coordinate transformation can be performed in two consecutive steps. Because the origin shift $\boldsymbol{p}$ 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):

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

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

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

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}$$

$$\text{with } \boldsymbol{Q} = \boldsymbol{P}^{-1} \text{ and } \boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p},$$
$$\text{thus } \boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p}). \quad (1.5.1.7)$$

The effect of a general change of the coordinate system $(\boldsymbol{P}, \boldsymbol{p})$ on the coefficients of a vector $\mathbf{r}$ is reduced to the linear transformation described by $\boldsymbol{P}$, 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

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

are often written in the following concise form:

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

1.5.2. Transformations of crystallographic quantities under coordinate transformations

BY H. WONDRATSCHEK AND M. I. AROYO

1.5.2.1. Covariant and contravariant quantities

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

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

where the notation $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ 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 $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$:

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

Quantities like the vector coefficients of any vector $\boldsymbol{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}$ 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 $\mathbf{a}, \mathbf{b}, \mathbf{c}$:

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