# 1.5. Transformations of coordinate systems

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It is in general advantageous to refer crystallographic objects and their symmetries to the most appropriate coordinate system. The best coordinate system may be different for different steps of the calculations and for different objects which have to be considered simultaneously. Therefore, a change of the origin and/or the basis are frequently necessary when treating crystallographic problems, for example in the study of phase-transition phenomena, or in the comparison of crystal structures described with respect to different coordinate systems.

## 1.5.1. Origin shift and change of the basis[1]

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### 1.5.1.1. Origin shift

Let a coordinate system be given with a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and an origin $O$. Referred to this coordinate system, the column of coordinates of a point $X$ is $\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ and the corresponding vector is $\mathbf{x} = x_1\mathbf{a} + x_2\mathbf{b} + x_3\mathbf{c}$. Referred to a new coordinate system, specified by the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and the origin $O'$, the column of coordinates of the point $X$ is $\boldsymbol{x}' = \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$. Let $\boldsymbol{p} = \overrightarrow{OO'} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$ be the column of coefficients for the vector $\mathbf{p}$ from the old origin $O$ to the new origin $O'$, see Fig. 1.5.1.1.

For the columns $\boldsymbol{p} + \boldsymbol{x}' = \boldsymbol{x}$ holds, *i.e.*

$$\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{p} \quad \text{or} \quad \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} x_1 - p_1 \\ x_2 - p_2 \\ x_3 - p_3 \end{pmatrix}. \tag{1.5.1.1}$$

This can be written in the formalism of matrix–column pairs (*cf.* Section 1.2.2.3 for details of the matrix–column formalism) as

$$\boldsymbol{x}' = (\boldsymbol{I}, -\boldsymbol{p})\boldsymbol{x} \quad \text{or} \quad \boldsymbol{x}' = (\boldsymbol{I}, \boldsymbol{p})^{-1}\boldsymbol{x}, \tag{1.5.1.2}$$

where $(\boldsymbol{I}, \boldsymbol{p})$ represents the translation corresponding to the vector $\mathbf{p}$ of the origin shift.

The vector $\mathbf{r}$ determined by the points $X$ and $Y$ (also known as a 'distance vector'), $\mathbf{x} + \mathbf{r} = \mathbf{y}$ (*cf.* Fig. 1.5.1.1), and thus with coefficients

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix},$$

shows a different transformation behaviour under the origin shift. From the diagram one reads the equations $\mathbf{p} + \mathbf{x}' = \mathbf{x}$, $\mathbf{x} + \mathbf{r} = \mathbf{y}$, $\mathbf{x}' + \mathbf{r} = \mathbf{y}'$, and thus

$$\mathbf{r} = \mathbf{y}' - \mathbf{x}' = \mathbf{y} - \mathbf{x}, \tag{1.5.1.3}$$

*i.e.* the vector coefficients of $\mathbf{r}$ are not affected by the origin shift.

*Example*

The description of a crystal structure is closely related to its space-group symmetry: different descriptions of the underlying space group, in general, result in different descriptions of the crystal structure. This example illustrates the comparison of two structure descriptions corresponding to different origin choices of the space group.

To compare the two structures it is not only necessary to apply the origin-shift transformation but also to adjust the selection of the representative atoms of the two descriptions.

In the Inorganic Crystal Structure Database (2012) (abbreviated as ICSD) one finds the following two descriptions of the mineral zircon $ZrSiO_4$:

(*a*) Wyckoff & Hendricks (1927), ICSD No. 31101, space group $I4_1/amd = D_{4h}^{19}$, No. 141, cell parameters $a$ = 6.61 Å, $c$ = 5.98 Å.

The coordinates of the atoms in the unit cell are (normalized so that $0 \le x_i < 1$):

| | | |
|---|---|---|
| Zr: | 4*a* | 0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{4}$ [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+] |
| Si: | 4*b* | 0, 0, $\frac{1}{2}$; 0, $\frac{1}{2}$, $\frac{3}{4}$ [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+] |
| O: | 16*h* | 0, 0.2, 0.34; 0.5, 0.3, 0.84; 0.8, 0.5, 0.59; 0.7, 0, 0.09; 0.5, 0.2, 0.41; 0, 0.3, 0.91; 0.7, 0.5, 0.16; 0.8, 0, 0.66 [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+]. |

The coordinates of Zr and Si atoms indicate that the space-group setting corresponds to the origin choice 1 description of $I4_1/amd$ given in this volume, *i.e.* origin at $\bar{4}m2$ (*cf.* the space-group tables for $I4_1/amd$ in Chapter 2.3).

(*b*) Krstanovic (1958), ICSD No. 45520, space group $I4_1/amd = D_{4h}^{19}$, No. 141, cell parameters $a$ = 6.6164 (5) Å, $c$ = 6.0150 (5) Å.

The coordinates of the atoms in the unit cell are (normalized so that $0 \le x_i < 1$):

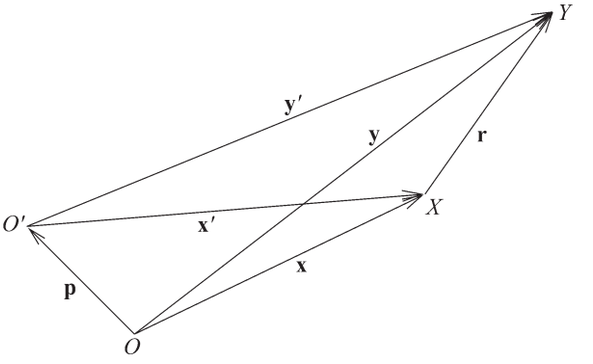


**Figure 1.5.1.1**
The coordinates of the points $X$ (or $Y$) with respect to the old origin $O$ are $\boldsymbol{x}$ ($\boldsymbol{y}$), and with respect to the new origin $O'$ they are $\boldsymbol{x}'$ ($\boldsymbol{y}'$). From the diagram one reads $\mathbf{p} + \mathbf{x}' = \mathbf{x}$ and $\mathbf{p} + \mathbf{y}' = \mathbf{y}$.

[1] With Table 1.5.1.1 and Figs. 1.5.1.2 and 1.5.1.5–1.5.1.10 by H. Arnold.

| | | |
|---|---|---|
| Zr: | 4*a* | $0, \frac{3}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$ [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$] |
| Si: | 4*b* | $0, \frac{1}{4}, \frac{3}{8}$; $0, \frac{3}{4}, \frac{5}{8}$ [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$] |
| O: | 16*h* | 0, 0.067, 0.198; 0.5, 0.933, 0.698; 0.183, 0.75, 0.448; 0.317, 0.25, 0.948; 0.5, 0.067, 0.302; 0, 0.933, 0.802; 0.317, 0.75, 0.052; 0.183, 0.25, 0.552 [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$]. |

The structure is described with respect to the origin choice 2 setting of $I4_1/amd$ specified in this volume as 'Origin at centre $(2/m)$ at $0, \frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$' (*cf.* the space-group tables for $I4_1/amd$ in Chapter 2.3).

In order to compare the different structure descriptions, the atomic coordinates of the origin choice 1 description are to be transformed to 'Origin at centre $2/m$', *i.e.* origin choice 2.

Origin choice 2 has coordinates $0, \frac{1}{4}, \frac{1}{8}$ referred to origin choice 1. Therefore, the change of coordinates consists of *subtracting* $\boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{4} \\ \frac{1}{8} \end{pmatrix}$ from the origin choice 1 values, *i.e.* leave the $x$ coordinate unchanged, add $\frac{1}{4} = 0.25$ to the $y$ coordinate and subtract $\frac{1}{8} = 0.125$ from the $z$ coordinate [*cf.* equation (1.5.1.1)].

The transformed and normalized coordinates (so that $0 \leq x_i < 1$) are

(i) Zr: 4*a* $0, \frac{1}{4}, \frac{7}{8}$; $0, \frac{3}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{1}{4}, \frac{5}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$;

(ii) Si: 4*b* $0, \frac{1}{4}, \frac{3}{8}$; $0, \frac{3}{4}, \frac{5}{8}$; $\frac{1}{2}, \frac{1}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{7}{8}$;

(iii) O: 16*h* $0, 0.20 + 0.25, 0.34 - 0.125 = 0, 0.45, 0.215$.

This oxygen atom obviously does not correspond to the representative 0, 0.067, 0.198 given by Krstanovic (1958), but by adding the centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ it is seen to correspond to the second position with coordinates 0.5, 0.933, 0.698. The transformed (and normalized) coordinates of the rest of the oxygen atoms in the unit cell are:

0.5, 0.55, 0.715; 0.8, 0.75, 0.465; 0.7, 0.25, 0.965;
0.5, 0.45, 0.285; 0, 0.55, 0.785; 0.7, 0.75, 0.035;
0.8, 0.25, 0.535;

all also with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$. The difference in the coordinates of the two descriptions could be explained by the difference in the accuracy of the two refinements.

### 1.5.1.2. Change of the basis

A change of the basis is described by a $(3 \times 3)$ matrix:

$$\boldsymbol{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}.$$

The matrix $\boldsymbol{P}$ relates the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ to the old basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ according to

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$
$$= (\mathbf{a}P_{11} + \mathbf{b}P_{21} + \mathbf{c}P_{31},\ \mathbf{a}P_{12} + \mathbf{b}P_{22} + \mathbf{c}P_{32},\ \mathbf{a}P_{13} + \mathbf{b}P_{23} + \mathbf{c}P_{33}). \quad (1.5.1.4)$$

The matrix $\boldsymbol{P}$ is often referred to as the *linear part* of the coordinate transformation and it describes a change of direction and/or length of the basis vectors. It is preferable to choose the matrix $\boldsymbol{P}$ in such a way that its determinant is positive: a negative determinant of $\boldsymbol{P}$ implies a change from a right-handed coordinate system to a left-handed coordinate system or *vice versa*. If $\det(\boldsymbol{P}) = 0$, then the new vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ are linearly dependent, *i.e.* they do not form a complete set of basis vectors.

For a point $X$ (*cf.* Fig. 1.5.1.1), the vector $\overrightarrow{OX} = \mathbf{x}$ is

$$\mathbf{x} = \mathbf{a}x_1 + \mathbf{b}x_2 + \mathbf{c}x_3 = \mathbf{a}'x_1' + \mathbf{b}'x_2' + \mathbf{c}'x_3' \text{ or}$$
$$\mathbf{x} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = (\mathbf{a}', \mathbf{b}', \mathbf{c}') \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}.$$

By inserting equation (1.5.1.4) one obtains

$$\mathbf{x} = (\mathbf{a}', \mathbf{b}', \mathbf{c}') \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$$

or

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix},$$

*i.e.* $\boldsymbol{x} = \boldsymbol{P}\boldsymbol{x}'$ or $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} = (\boldsymbol{P}, \boldsymbol{o})^{-1}\boldsymbol{x}$, which is often written as

$$\boldsymbol{x}' = \boldsymbol{Q}\boldsymbol{x} = (\boldsymbol{Q}, \boldsymbol{o})\boldsymbol{x}. \quad (1.5.1.5)$$

Here the inverse matrix $\boldsymbol{P}^{-1}$ is designated by $\boldsymbol{Q}$, while $\boldsymbol{o}$ is the $(3 \times 1)$ column vector with zero coefficients. [Note that in equation (1.5.1.4) the sum is over the row (first) index of $\boldsymbol{P}$, while in equation (1.5.1.5), the sum is over the column (second) index of $\boldsymbol{Q}$.]

A selected set of transformation matrices $\boldsymbol{P}$ and their inverses $\boldsymbol{P}^{-1} = \boldsymbol{Q}$ that are frequently used in crystallographic calculations are listed in Table 1.5.1.1 and illustrated in Figs. 1.5.1.2 to 1.5.1.10.

*Example*

Consider an *F*-centred cell with conventional basis $\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F$ and a corresponding primitive cell with basis $\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P$, *cf.* Fig. 1.5.1.4. The transformation matrix $\boldsymbol{P}$ from the conventional basis to a primitive basis can either be deduced from Fig. 1.5.1.4 or can be read directly from Table 1.5.1.1: $\mathbf{a}_P = \frac{1}{2}(\mathbf{b}_F + \mathbf{c}_F)$, $\mathbf{b}_P = \frac{1}{2}(\mathbf{a}_F + \mathbf{c}_F)$, $\mathbf{c}_P = \frac{1}{2}(\mathbf{a}_F + \mathbf{b}_F)$, which in matrix notation is

$$(\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P) = (\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F)\boldsymbol{P} = (\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F) \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}.$$

The inverse matrix $\boldsymbol{P}^{-1} = \boldsymbol{Q}$ is also listed in Table 1.5.1.1 or can be deduced from Fig. 1.5.1.4. It is the matrix that describes the conventional basis vectors $\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F$ by linear combinations of $\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P$: $\mathbf{a}_F = -\mathbf{a}_P + \mathbf{b}_P + \mathbf{c}_P$, $\mathbf{b}_F = \mathbf{a}_P - \mathbf{b}_P + \mathbf{c}_P$, $\mathbf{c}_F = \mathbf{a}_P + \mathbf{b}_P - \mathbf{c}_P$, or

$$(\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F) = (\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P)\boldsymbol{P}^{-1} = (\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P) \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

Correspondingly, the point coordinates transform as