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 $0 \le x_i < 1$):

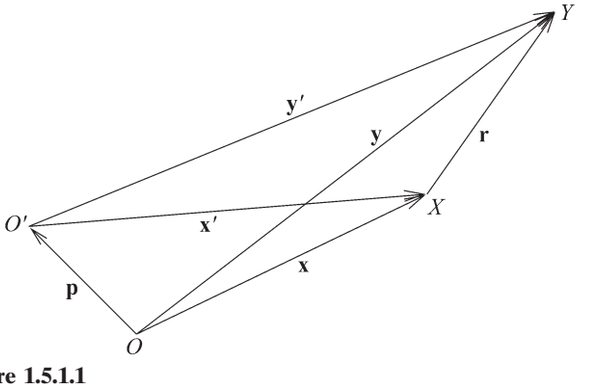

Figure 1.5.1.1
The coordinates of the points X (or Y) with respect to the old origin O are $\boldsymbol{x}$ ($\boldsymbol{y}$), and with respect to the new origin O' they are $\boldsymbol{x}'$ ($\boldsymbol{y}'$). From the diagram one reads $\mathbf{p} + \mathbf{x}' = \mathbf{x}$ and $\mathbf{p} + \mathbf{y}'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

[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.

references