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Confirmation of the Handedness of Transformed Unit Cell

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變換된 Unit Cell의 Handedness 確認

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The crystallographic problem: There are seven three-dimensional coordinate systems/unit cells which are useful in describing crystals and which are the basis for their classification. They function as a coordinate system to which the actual structure is referred. The three coordinate axes are termed x, y, and z and are ordinarily chosen to form a right-handed system.

Almost two-thirds of the 230 space groups can be expressed in different ways according to the setting of unit-cell axis,[1] and besides if non-standard space groups are obtained by, for example, X-ray photographic methods or four-circle diffractometry, it is sometimes desirable to transform them into standard space groups by means of crystallographic axis interchange or axis transformation or reversion of the sense of the crystallographic axes or whatever. In all cases the right-handed system must be maintained. Therefore, whenever a unit cell is transformed, the handedness of the newly obtained unit cell must be confirmed.

Method of solution:

(1) Resolution of triclinic axes into their components in an orthonormal coordinate system.

Let a, b, c, α, β, γ be triclinic cell data and $\vec{i}$, $\vec{j}$, $\vec{k}$ be orthonormal axial unit vectors and both of them be right-handed systems with origin at o.

Assuming $\vec{i}$ parallel to $\vec{a}$, and $\vec{j}$ is in (a, b) plane and perpendicular to $\vec{a}$, and $\vec{k}$ is perpendicular to both $\vec{i}$ and $\vec{j}$, the following direction cosines are obtained.

$l_1=\cos(\angle aoi)=\cos 0=1$
$l_2=\cos(\angle aoj)=\cos 90=0$
$l_3=\cos(\angle aok)=\cos 90=0$
$m_1=\cos(\angle boi)=\cos\gamma$
$m_2=\cos(\angle boj)=\cos(\gamma-90)=\sin\gamma$
$m_3=\cos(\angle bok)=\cos 90=0$
$n_1=\cos(\angle coi)=\cos\beta$
$n_2=\cos(\angle coj)$
$n_3=\cos(\angle cok)$.

Then each of the unit vectors $\frac{\vec{a}}{a}, \frac{\vec{b}}{b}, \frac{\vec{c}}{c}$ can be written in terms of the vector sum of the $\vec{i}$, $\vec{j}$ and $\vec{k}$ components as follows:

$$\frac{\vec{a}}{a}=l_1\vec{i}+l_2\vec{j}+l_3\vec{k}$$
$$\frac{\vec{b}}{b}=m_1\vec{i}+m_2\vec{j}+m_3\vec{k}$$
$$\frac{\vec{c}}{c}=n_1\vec{i}+n_2\vec{j}+n_3\vec{k}\,, \tag{1}$$

where the n_2 can be obtained from the scalar product of $\frac{\vec{b}}{b}\cdot\frac{\vec{c}}{c}$

$$\frac{\vec{b}}{b}\cdot\frac{\vec{c}}{c}=\cos\alpha=(m_1\vec{i}+m_2\vec{j}+m_3\vec{k})\cdot(n_1\vec{i}+n_2\vec{j}+n_3\vec{k})$$
$$=m_1n_1+m_2n_2+m_3n_3=\cos\gamma\cos\beta+\sin\gamma\, n_2$$
$$n_2=\frac{\cos\alpha-\cos\gamma\cos\beta}{\sin\gamma}$$

and the n_3 from the scalar product of $\frac{\vec{c}}{c}\cdot\frac{\vec{c}}{c}$

$$\frac{\vec{c}}{c}\cdot\frac{\vec{c}}{c}=1=n_1^2+n_2^2+n_3^2=\cos^2\beta+n_2^2+n_3^2$$

$$n_3=(\sin^2\beta-n_2^2)^{0.5}.$$

Substitution of the direction cosines into Eq. (1) gives:

$$\begin{pmatrix}\vec{a}/a\\ \vec{b}/b\\ \vec{c}/c\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ \cos\gamma & \sin\gamma & 0\\ \cos\beta & n_2 & n_3\end{pmatrix}\begin{pmatrix}\vec{i}\\ \vec{j}\\ \vec{k}\end{pmatrix}.$$

Thus the triclinc axes can be expressed in terms of the orthonormal axes:

$$\begin{pmatrix}\vec{a}\\ \vec{b}\\ \vec{c}\end{pmatrix}=\begin{pmatrix}a & 0 & 0\\ b\cos\gamma & b\sin\gamma & 0\\ c\cos\beta & c\,n_2 & c\,n_3\end{pmatrix}\begin{pmatrix}\vec{i}\\ \vec{j}\\ \vec{k}\end{pmatrix}$$

$$=\begin{pmatrix}\vec{i}a\\ \vec{i}b\cos\gamma+\vec{j}b\sin\gamma\\ \vec{i}c\cos\beta+\vec{j}c\,n_2+\vec{k}c\,n_3\end{pmatrix} \quad (2)$$

(2) Volume of a triclinic cell

The volume of a parallelepiped, whose three intersecting edges are $\vec{a}$, $\vec{b}$ and $\vec{c}$, is calculated using the triple scalar product $\vec{a}\times\vec{b}\cdot\vec{c}$ where the dot and cross may be interchanged. The triple scalar product can be expressed by way of determinant in a simple way:

$$V=\vec{a}\times\vec{b}\cdot\vec{c}=\begin{vmatrix}a_x & a_y & a_z\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{vmatrix} \quad (3)$$

where the elements of the determinant are components of $\vec{a}$, $\vec{b}$ and $\vec{c}$ projected to each axis of an orthonormal coordinate system.

Substitution of Eq. (2) into Eq. (3) gives the volume of the triclinic cell:

$$V=\begin{vmatrix}a & 0 & 0\\ b\cos\gamma & b\sin\gamma & 0\\ c\cos\beta & c\,n_2 & c\,n_3\end{vmatrix}=a\,b\,c\,n_3\sin\gamma$$

$$=abc(1-\sin^2\alpha-\sin^2\beta-\sin^2\gamma-2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

(3) Confirmation of the handedness

Recalling that an interchange of rows changes the sign of a determinant of Eq. (3), we can easily write out the six products. If the order of the interchange of rows is cyclic, all such triple scalar products are equal. If the order of the interchange of rows is non-cyclic, however, another set all equal to each other but the negatives of the first set is obtained:

$$+\vec{a}\times\vec{b}\cdot\vec{c}=+\vec{b}\times\vec{c}\cdot\vec{a}=+\vec{c}\times\vec{a}\cdot\vec{b}$$
$$=-\vec{b}\times\vec{a}\cdot\vec{c}=-\vec{c}\times\vec{b}\cdot\vec{a}=-\vec{a}\times\vec{c}\cdot\vec{b}, \quad (4)$$

where the positive signs indicate the right-handed systems while the negative signs signify the left-handed ones meaning non-cyclical axis interchange.

The fact about the determinant shown by Eq. (4) can be used as a criterion judging the handedness of a unit cell.

As an example, let us transform the unit cell given by Eq. (2) using a transformation matrix $\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}$, which signifies obviously a non-cyclical axis interchange.

Then the new cell axes a', b' c' are

$$\begin{pmatrix}\vec{a}'\\ \vec{b}'\\ \vec{c}'\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\vec{a}\\ \vec{b}\\ \vec{c}\end{pmatrix}$$

$$=\begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\vec{i}a\\ \vec{i}b\cos\gamma+\vec{j}b\sin\gamma\\ \vec{i}c\cos\beta+\vec{j}c\,n_2+\vec{k}c\,n_3\end{pmatrix}$$

and the volume V' of the new unit cell is

$$V=\begin{vmatrix}a & 0 & 0\\ -b\cos\gamma & -b\sin\gamma & 0\\ c\cos\beta & c\,n_2 & cn_3\end{vmatrix}=-a\,b\,c\,n_3\sin\gamma.$$

As expected, the volume has a negative sign.

Now one can make a general transformation equation.

Applying a general transformation matrix given below to Eq. (2)

$$\begin{pmatrix} p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \\ s_1 & s_2 & s_3 \end{pmatrix},$$

the transformed cell parameters become:

$$\begin{pmatrix} \vec{a}' \\ \vec{b}' \\ \vec{c}' \end{pmatrix} = \begin{pmatrix} p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \\ s_1 & s_2 & s_3 \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} = \begin{pmatrix} p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \\ s_1 & s_2 & s_3 \end{pmatrix} \begin{pmatrix} \vec{i}a \\ \vec{i}b\cos\gamma + \vec{j}b\sin\gamma \\ \vec{i}c\cos\beta + \vec{j}c\, n_2 + \vec{k}c\, n_3 \end{pmatrix}$$

$$\begin{pmatrix} \vec{a}' \\ \vec{b}' \\ \vec{c}' \end{pmatrix} = \begin{pmatrix} p_1\vec{i}a + p_2\vec{i}b\cos\gamma + p_2\vec{j}b\sin\gamma + p_3\vec{i}c\cos\beta + p_3\vec{j}cn_2 + p_3\vec{k}cn_3 \\ q_1\vec{i}a + q_2\vec{i}b\cos\gamma + q_2\vec{j}b\sin\gamma + q_3\vec{i}c\cos\beta + q_3\vec{j}cn_2 + q_3\vec{k}cn_3 \\ s_1\vec{i}a + s_2\vec{i}b\cos\gamma + s_2\vec{j}b\sin\gamma + s_3\vec{i}c\cos\beta + s_3\vec{j}cn_2 + s_3\vec{k}cn_3 \end{pmatrix}$$

$$= \begin{pmatrix} \vec{i}(p_1a + p_2b\cos\gamma + p_3c\cos\beta) + \vec{j}(p_2b\sin\gamma + p_3cn_2) + \vec{k}p_3cn_3 \\ \vec{i}(q_1a + q_2b\cos\gamma + q_3c\cos\beta) + \vec{j}(q_2b\sin\gamma + q_3cn_2) + \vec{k}q_3cn_3 \\ \vec{i}(s_1a + s_2b\cos\gamma + s_3c\cos\beta) + \vec{j}(s_2b\sin\gamma + s_3cn_2) + \vec{k}s_3cn_3 \end{pmatrix}$$

Accordingly the magnitudes of the transformed unit cell parameters are:

$$\left.\begin{array}{l} a' = [(p_1a + p_2b\cos\gamma + p_3c\cos\beta)^2 + (p_2b\sin\gamma + p_3cn_2)^2 + (p_3cn_3)^2]^{0.5} \\ b' = [(q_1a + q_2b\cos\gamma + q_3c\cos\beta)^2 + (q_2b\sin\gamma + q_3cn_2)^2 + (q_3cn_3)^2]^{0.5} \\ c' = [(s_1a + s_2b\cos\gamma + s_3c\cos\beta)^2 + (s_2b\sin\gamma + s_3cn_2)^2 + (s_3cn_3)^2]^{0.5} \\ \alpha' = \arccos[((q_1a+q_2b\cos\gamma+q_3c\cos\beta)(s_1a+s_2b\cos\gamma+s_3c\cos\beta) \\ \quad +(q_2b\sin\gamma+q_3cn_2)(s_2b\sin\gamma+s_3cn_2)+(q_3cn_3)(s_3cn_3))/(b'c')] \\ \beta' = \arccos[((p_1a+p_2b\cos\gamma+p_3c\cos\beta)(s_1a+s_2b\cos\gamma+s_3c\cos\beta) \\ \quad +(p_2b\sin\gamma+p_3cn_2)(s_2b\sin\gamma+s_3cn_2)+(p_3cn_3)(s_3cn_3))/(c'a')] \\ \gamma' = \arccos[((p_1a+p_2b\cos\gamma+p_3c\cos\beta)(q_1a+q_2b\cos\gamma+q_3c\cos\beta) \\ \quad +(p_2b\sin\gamma+p_3cn_2)(q_2b\sin\gamma+q_3cn_2)+(p_3cn_3)(q_3cn_3))/(a'b')] \end{array}\right\} \quad (5)$$

and the volume of the transformed cell can be calculated by the determinant of components projected on the orthonormal coordinate axes:

$$V = \begin{vmatrix} (p_1a+p_2b\cos\gamma+p_3c\cos\beta) & (p_2b\sin\gamma+p_3cn_2) & p_3cn_3 \\ (q_1a+q_2b\cos\gamma+q_3c\cos\beta) & (q_2b\sin\gamma+q_3cn_2) & q_3cn_3 \\ (s_1a+s_2b\cos\gamma+s_3c\cos\beta) & (s_2b\sin\gamma+s_3cn_2) & s_3cn_3 \end{vmatrix} \quad (6)$$

The program RLVOLUME calculates the cell parameters given by Eq. (5) and the volume given by Eq. (6).
If the program RLVOLUME gives a negative volume, the transformation matrix must be corrected so as

to get a right-handed system.

Documentation and availability: The source code written in Fortran 95 and an execution file executable on a PC can be downloaded from the World Wide Web site http://www.cnu.ac.kr/~insuh/

Reference

1) Henry, N. F. M. and Lonsdale, K. International Table for X-ray Crystallography, Vol. 1. 545-553. Birmingham: Kynoch Press. (present distributors: Klumer Academic Publishers, Dordrecht.) (1969).