Coordinate Transformations in Crystallography

Jon Cooper (March/April 2021)

1 The basis set

The normal convention is for the X-axis to be parallel with the **a** axis of the unit cell and for the Y-axis to be oriented in the **ab** plane. In the figure below (Fig. 1), the X-axis is therefore pointing towards the viewer exactly parallel with the **a** vector, shown as ⓐ. The Y-axis is pointing upwards and the Z-axis

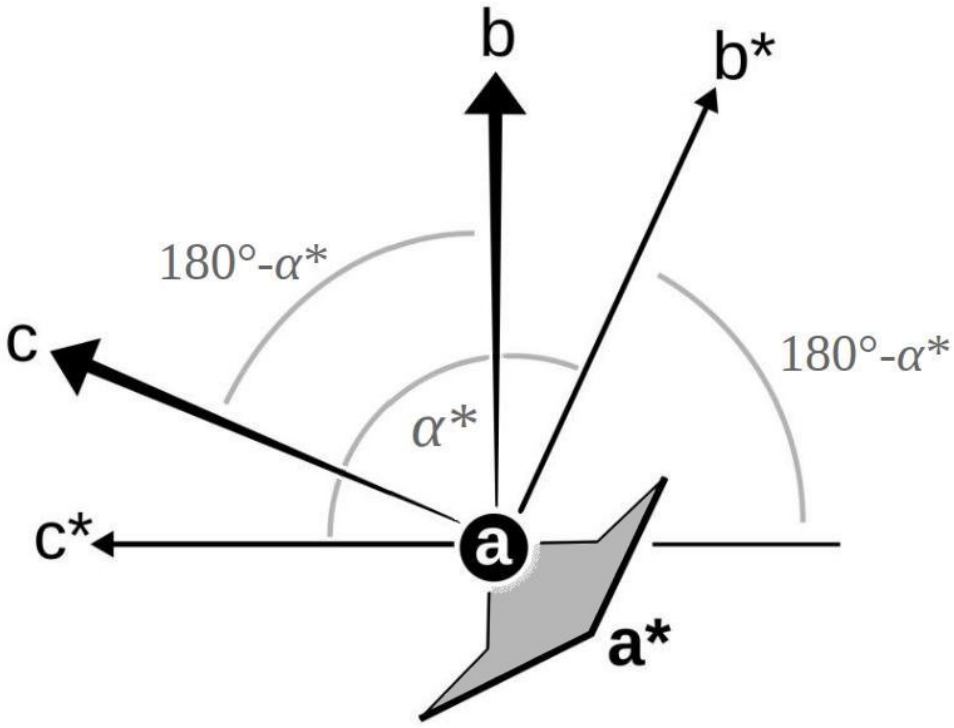

Figure 1: The real and reciprocal lattice vectors as viewed from the direction of the unit cell vector **a** which is pointing towards the viewer and is coincident with the Cartesian X-axis. The Y-axis points vertically upwards in the plane of the page behind **b** and the Z-axis is coincident with **c***.

is pointing horizontally to the left. In the completely general case of a triclinic crystal where **a**, **b** and **c** are not orthogonal, the **b** and **c** vectors will pointing out of the plane of the page. Normally, the triclinic unit cell is chosen with the unit cell angles acute, although it is allowed for all of them to be obtuse. The latter would mean that **b** and **c** would be pointing away from the viewer, which is a bit of a pain to draw, so we will assume that α, β and γ are acute, which allows all the unit cell vectors to point towards the viewer. The positive

direction of the rectangular Cartesian Y-axis will be behind the **b** vector (as drawn) and lie in the plane of the page and the Z-axis will be parallel with **c*** as drawn. For orthorhombic, tetragonal or cubic unit cells, **b** and **b*** will coincide exactly in the plane of the page, as will **c** and **c***. The **a** and **a*** axes which are pointing towards the viewer will also coincide for these crystal systems. However, in the general triclinic case, they do not, and are therefore drawn separately. The **a*** axis is shown pointing towards the viewer in the lower-right hand direction. Note that **a*** is orthogonal to **b** and **c** and likewise for the other combinations *i.e.* **b*** is orthogonal to **a** and **c**, and **c*** is orthogonal to **a** and **b**. Accordingly, **a** is orthogonal to **b*** and **c***, **b** is orthogonal to **a*** and **c***, and **c** is orthogonal to **a*** and **b***. All the axes are drawn in the usual right-handed convention. If any of this is not making sense, the reader must go back to a fundamental crystallography text book.

Looking down the **a** vector we see that the angle between **b*** and **c*** is, of course, α^*. This is the actual angle between the **b*** and and **c*** vectors in the plane of the page. If we look at the angles on the plane of the page and remember that **c*** is at right-angles to the plane defined by vectors **a** and **b** and that **b*** is at right-angles to the plane defined by vectors **a** and **c**, with a bit of basic trigonometry we can show that the angle between the plane formed by vectors **a** and **b** and the plane formed by vectors **a** and **c** is 180°-α^*. This is the angle between these two planes measured in the plane of the page. It is important to note that this is not the same as the angle between the **b** and **c** vectors in three dimensions (which is α) since these vectors are projecting out of the page. However, looking exactly along the **a** vector they appear to be separated by an angle of 180°-α^*. We can imagine looking at the earth from above the north pole and if the vectors **b** and **c** point from the centre of the earth towards two cities, then 180°-α^* would be the difference in their longitudes.

So if we consider the tip of the vector **a** as being the north pole, vectors **b** and **c** differ in longitude by 180°-α^*. Likewise, if we consider the tip of the **b** vector to be the north pole, vectors **a** and **c** would differ in longitude by 180°-β^* and with **c** as the polar axis, vectors **a** and **b** would differ in longitude by 180°-γ^*. Exactly the same arguments apply to the reciprocal lattice vectors, *e.g.* if the tip of the vector **a*** is taken as the north pole, vectors **b*** and **c*** differ in longitude by 180°-α. This is all quite tedious to write, but can be summarised by the following diagram (Fig. 2) showing the relationships between the real and reciprocal unit cell angles as spherical triangles.

This allows us to use spherical trigonometry to work out the reciprocal cell angles (α^*, β^* and γ^*) from the real unit cell angles (α, β and γ) and *vice versa*.

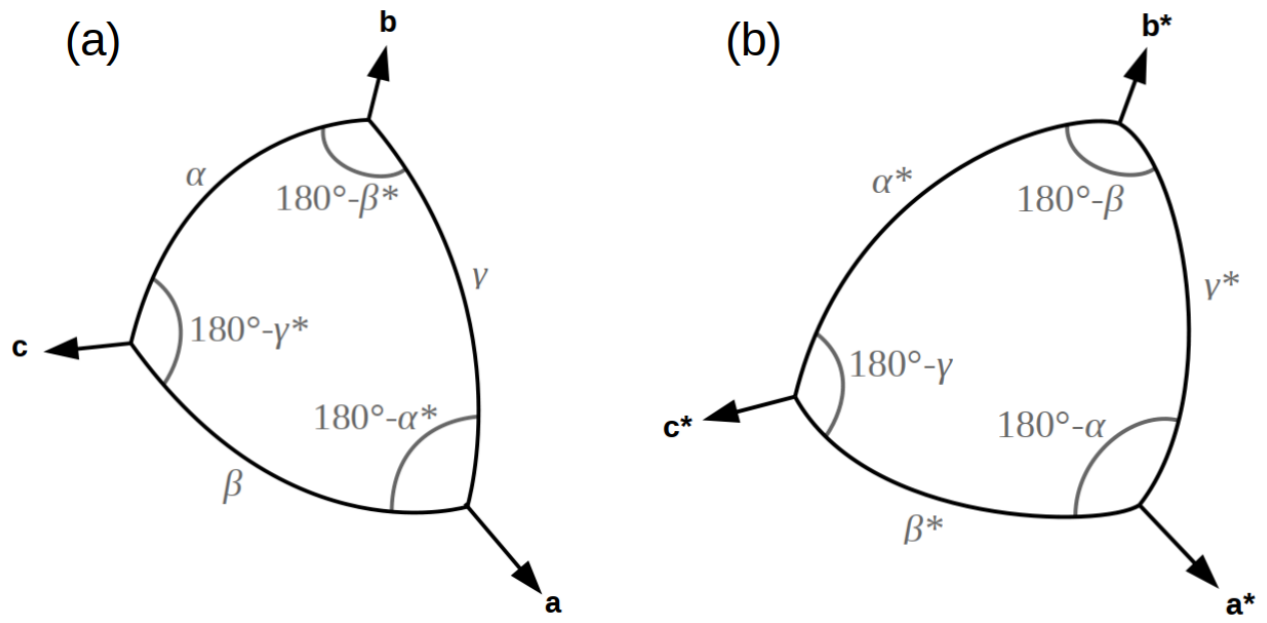

Figure 2: (a) The unit cell vectors **a**, **b** and **c** diverge from the origin (not shown) by angles α, β and γ in the manner shown. (b) The reciprocal lattice vectors **a***, **b*** and **c*** diverge by the angles α^*, β^* and γ^*. The curves indicate portions of great circles, *i.e.* circles which have their centres at the centre of a sphere on which they are drawn. This might sound obvious, but lines of constant latitude are (with the exception of the equator) not great circles since their centres align with the polar axis of the globe rather than the centre of the earth. Indeed, latitude lines other than the equator are called small circles. In contrast, all lines of constant longitude are great circles. Hence, we can see from (a) that if **a** is regarded as the polar axis, the longitudes of **b** and **c** differ by 180°-α^*. Likewise, from (b) we can see that if we treat **a*** as the polar axis, the longitudes of **b*** and **c*** differ by 180°-α.

2 Fundamental spherical trigonometry

With reference to Fig. 3 the following equations are true for all spherical triangles formed by the intersection of great circles. A great circle can be drawn between any two points on the surface of a sphere and represents the shortest possible distance between those points.

Spherical sine rule:

$$\frac{\sin(A)}{\sin(a)} = \frac{\sin(B)}{\sin(b)} = \frac{\sin(C)}{\sin(c)} \tag{1}$$

Spherical cosine rule:

$$\cos(a) = \cos(b)\cos(c) + \sin(b)\sin(c)\cos(A) \tag{2}$$

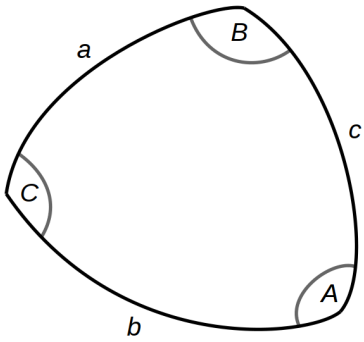

Figure 3: A general spherical triangle with sides a, b and c which are arcs formed by great circles. Note that a, b and c are actually the angles subtended by each arc at the centre of the sphere. A given arc defines a plane and the angles between these planes are shown in capital letters as A, B and C.

By comparison of Fig. 3 with Fig. 2(a) can use the sine rule to show the following:

$$\frac{\sin(180^\circ - \alpha^*)}{\sin(\alpha)} = \frac{\sin(180^\circ - \beta^*)}{\sin(\beta)} = \frac{\sin(180^\circ - \gamma^*)}{\sin(\gamma)} \tag{3}$$

or

$$\frac{\sin(\alpha^*)}{\sin(\alpha)} = \frac{\sin(\beta^*)}{\sin(\beta)} = \frac{\sin(\gamma^*)}{\sin(\gamma)} \tag{4}$$

Likewise the cosine rule gives us other relationships such as:

$$\cos(\alpha) = \cos(\beta)\cos(\gamma) + \sin(\beta)\sin(\gamma)\cos(180^\circ - \alpha^*) \tag{5}$$

or

$$\cos(\alpha) = \cos(\beta)\cos(\gamma) - \sin(\beta)\sin(\gamma)\cos(\alpha^*) \tag{6}$$

This is more useful than the sine rule since we can rearrange it as follows:

$$\cos(\alpha^*) = \frac{\cos(\beta)\cos(\gamma) - \cos(\alpha)}{\sin(\beta)\sin(\gamma)} \tag{7}$$

This allows us to determine α^* unambiguously from the real unit cell angles since it must be in the range 0 - 180°. Of course, equivalent expressions can be derived for β^* and γ^*.

3 Application to unit cell vectors

We have seen how the relative directions of the unit cell vectors can be conveniently described by spherical trigonometry but our aim is to describe their

orientation with respect to an orthonormal system of axes. In the below figure (Fig. 4) we show how this is done.

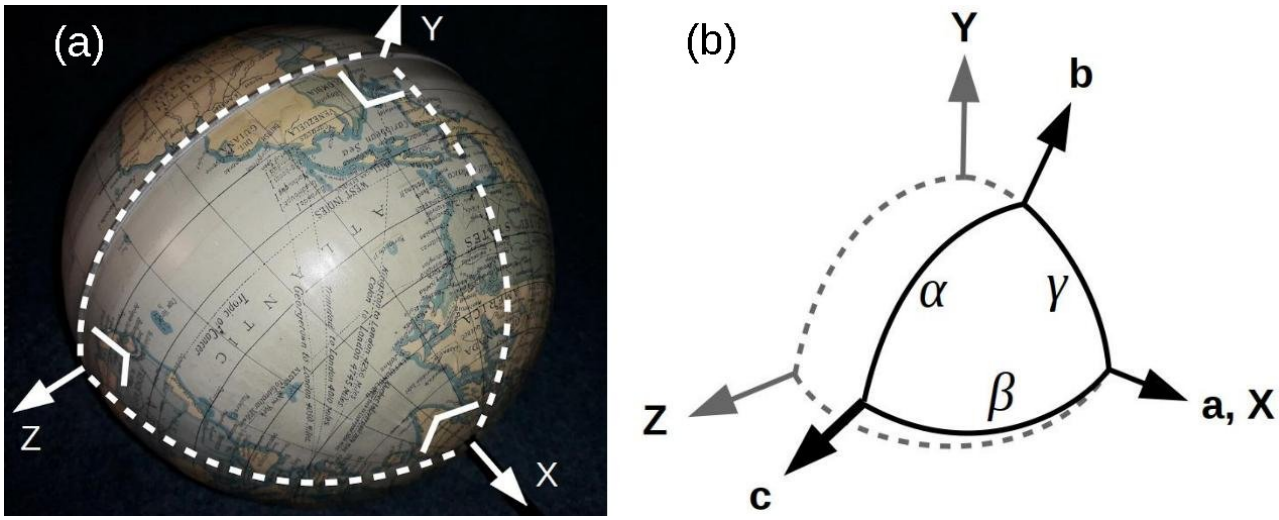

Figure 4: In (a) a system of orthonormal axes with its origin at the earth's centre is shown. Our view is from above the Atlantic with X as the polar axis (pointing to the lower right) while Y and Z are equatorial. The dashed lines on the globe indicate 90° arcs of great circles, *i.e.* they subtend 90° angles at the centre of the earth and thus enclose 1/8 of the sphere, or an *octant*. These arcs lie in planes which are at 90° to one another, indicated as right angle symbols at the corners of the triangle. Hence, the sum of the angles for this triangle is 270°, which is perfectly fine on the surface of a sphere! The right-hand side (b) shows the convention for aligning crystallographic unit cell vectors with orthonormal axes. The grey dashed lines indicate 90° arcs, as for the octant in (a). Unit cell vector **a** is aligned with the X-axis while **b** lies within the XY plane. Since these are both right-handed axial systems, the vector **c** points in a roughly similar direction to Z, but is oriented more towards the viewer in this case. Note that we chose a triclinic cell in which all the unit cell angles α, β and γ are acute (the corresponding great circles are labelled). This means that **b** and **c** emerge within the same octant as shown.

From Fig. 4(b) we can see that the situation with the **a** and **b** axes is relatively straightforward since **a** is parallel to X (*i.e.* it is at 90° to both Y and Z) and **b** is γ from **a**, 90°-γ from Y and 90° from Z. It is also clear that **c** is at an angle of β from X, however the angular distances of **c** from Y and Z are harder to determine and require use of the cosine rule. The appropriate triangulation is shown in Fig. 5.

The unknown angular distances that we require are shown as δ and ε in Fig. 5 and specify the angles that separate **c** from Y and Z, respectively. Considering the spherical triangle formed by X, Y and **c**, we can use the cosine rule to show:

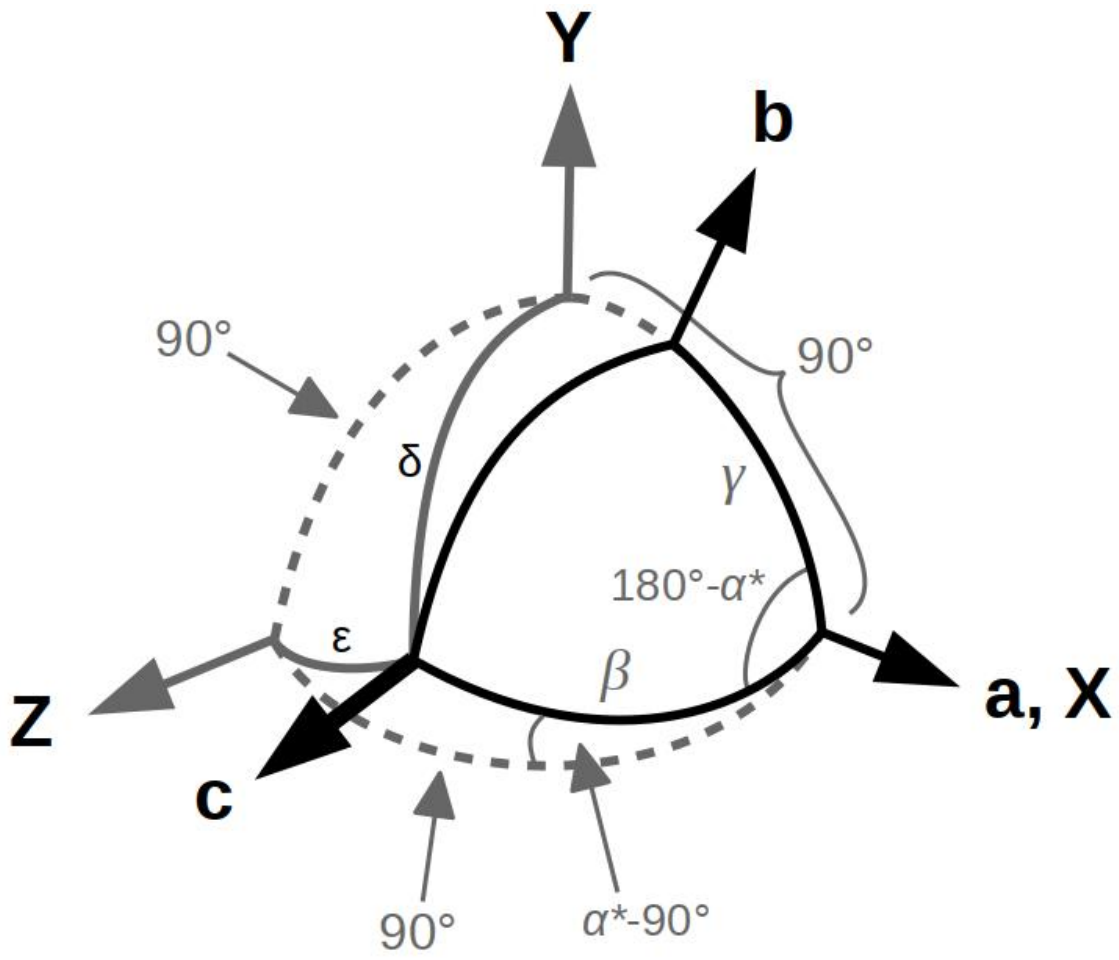

Figure 5: Spherical triangulation to determine inter-axial angles. Here Fig.4(b) has been redrawn showing more detail. The angles β and γ are known, and α^* can be calculated from equation 7. The two angles, δ and ε, which give the orientation of the **c** axis with respect to the orthonormal Y- and Z-axes, are given by equations (9) and (11). The vector **a** is parallel to X (*i.e.* is at 90° to both Y and Z) and **b** is γ from **a**, 90°-γ from Y and 90° from Z.

$$\cos(\delta) = \cos(\beta)\cos(90^\circ) + \sin(\beta)\sin(90^\circ)\cos(180^\circ - \alpha^*) \tag{8}$$

which can be simplified by basic trigonometry to:

$$\cos(\delta) = -\sin(\beta)\cos(\alpha^*) \tag{9}$$

Similarly, with the lowest spherical triangle shown in Fig. 5, which is formed by X, Z and **c**, we can show:

$$\cos(\varepsilon) = \cos(\beta)\cos(90^\circ) + \sin(\beta)\sin(90^\circ)\cos(\alpha^* - 90^\circ) \tag{10}$$

Since $\cos(-\theta)=\cos(\theta)$, $\cos(\alpha^*-90^\circ)=\cos(90^\circ-\alpha^*)$ and since $\cos(90^\circ-\theta)=\sin(\theta)$, $\cos(90^\circ-\alpha^*)=\sin(\alpha^*)$. Therefore equation (10) becomes:

$$\cos(\varepsilon)=\sin(\beta)\sin(\alpha^*) \tag{11}$$

The highlighted equations (9) and (11) are the crux of what comes next!

4 Converting from fractional to orthogonal coordinates and *vice versa*

If an atom is located at a fractional coordinate of x along the **a** axis, its coordinate on the X-axis would be ax. Since **a** is at right-angles to the Y- and Z-axes, the Y and Z values are independent of x.

If the atom has a fractional coordinate on the **b** axis of y, this has components on the X- and Y-axes but not Z since **b** is at right angles to this axis. The component of $y\mathbf{b}$ on the Y-axis is dictated by the angle between **b** and this axis. Reference to Fig. 5 shows that this component is given by simple trigonometry as $yb\cos(90°\text{-}\gamma)$ or $yb\sin(\gamma)$. Since **b** is not orthogonal to the X-axis, then $y\mathbf{b}$ has a component on this axis of $yb\cos(\gamma)$. Again, since **b** is orthogonal to Z, $y\mathbf{b}$ has no component on this axis.

The situation with **c** is that $z\mathbf{c}$ has components on all three orthonormal axes (X, Y and Z) which are, of course, dictated by their angular distance from **c**. Reference to Fig. 5 shows that these angles are β, δ and ε, respectively. The component of $z\mathbf{c}$ on X is therefore $zc\cos(\beta)$ and the components on Y and Z are $zc\cos(\delta)$ and $zc\cos(\varepsilon)$, respectively. Using equations (9) and (11) we can see that:

$$zc\cos(\delta) = -zc\sin(\beta)\cos(\alpha^*) \tag{12}$$

and

$$zc\cos(\varepsilon) = zc\sin(\beta)\sin(\alpha^*) \tag{13}$$

Summing these components on each of the orthonormal axes, we see that:

$$X = xa + yb\cos(\gamma) + zc\cos(\beta) \tag{14}$$

$$Y = yb\sin(\gamma) - zc\sin(\beta)\cos(\alpha^*) \tag{15}$$

$$Z = zc\sin(\beta)\sin(\alpha^*) \tag{16}$$

This has an elegant upper-triangular matrix representation as follows:

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} a & b\cos(\gamma) & c\cos(\beta) \\ 0 & b\sin(\gamma) & -c\sin(\beta)\cos(\alpha^*) \\ 0 & 0 & c\sin(\beta)\sin(\alpha^*) \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{17}$$

Hence, in order to orthogonalise a set of fractional coordinates, we need to calculate the terms in the 3x3 matrix. Since α, β and γ are known, the only unknowns are the cos and sin of α^* which can be calculated from equation (7) and from the relationship:

$$\sin(\theta) = \sqrt{1 - \cos^2(\theta)} \tag{18}$$

Given that the angle will be less than 180° by convention, $\sin(\theta)$ should be positive.

We can also obtain the fractional coordinates from the Cartesian ones by inversion of the 3x3 matrix above.

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} a & b\cos(\gamma) & c\cos(\beta) \\ 0 & b\sin(\gamma) & -c\sin(\beta)\cos(\alpha^*) \\ 0 & 0 & c\sin(\beta)\sin(\alpha^*) \end{pmatrix}^{-1} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} \tag{19}$$

This can be done by a maths library so will not be expanded further.

5 Closing remarks and references

There are other ways to orthogonalise fractional coordinates, *e.g.* to align **c** with the Z-axis and to have **b** coplanar with Y and Z. The spherical trigonometry of this system is derived at the start of Chapter 3 of ***Computing Methods in Crystallography*** **(Ed. J. S. Rollett), Pergamon Press, Oxford (1965)** ***pp.*** **22-3** and this derivation has simply been adapted here for the current convention of aligning **a** with X. An alternative derivation using dot products of **i**, **j** and **k** vectors, which avoids spherical trigonometry altogether, is given by other authors, including **J. W. Jeffery** in ***Methods in X-ray Crystallography*****, Academic Press, London (1971)** ***pp.*** **333-4**. Some derivations involve calculating the unit cell volume (*e.g.* this one at ruppweb.org).

There are other potential complications *e.g.* with monoclinic systems, some workers preferred to align **b** with Z so that the only non-90° angle (or *unique angle*), β, is shown in plotted map-sections. This involves a cyclic permutation of the orthonormal axes, giving Z, X, Y which are aligned with **c**, **a** and **b**, respectively, *i.e.* Y becomes the *slowest-changing axis*. This helps with calculating the map by fast Fourier transform, however, since β is not fixed at 90°, there is a choice of whether to orient **a** exactly with X or **c** with Z.

For completeness, the CCP4 program PDBSET (P. Evans, MRC LMB, Cambridge, September 1992) lists the following possible combinations:

NCODE	X	Y	Z
1	**a**	**c* × a**	**c***
2	**b**	**a* × b**	**a***
3	**c**	**b* × c**	**b***
4	**a+b**	**c* × (a + b)**	**c***
5	**a***	**c × a***	**c**
6	**a**	**b***	**a × b***
7	**a***	**b**	**a* × b**

NCODE 1 is the orthogonalisation convention we have described in detail here (*i.e.* the Protein Data Bank (www.rcsb.org) or PDB system), 3 is occassionally used for monoclinic cells since it aligns **b** with Z (and **c** with X), 5 is the system mentioned above due to Rollett (1965) and 7 is that used by the program TNT (Tronrud, D. E., Ten Eyck, L. F. & Matthews, B. W. (1987). *Acta Crystallogr. A*, **43**, 489-501).

Note that plane normals are indicated by vector cross-products in this table and, again, if that doesn't make sense, then a fundamental textbook must be referred to.

While chemical X-ray structures are usually stored as fractional coordinates (in Crystallographic Information Files or CIF's for short), the larger scale of biological macromolecules means that it would not make efficient use of computer memory to store them in this manner. Consequently they are stored as orthogonal Å coordinates and regenerating the fractional coordinates therefore requires knowledge of the orthogonalisation convention. The NCODE 1 scheme (row with highlighted text in the table) is the standard adopted for both PDB and macromolecular CIF (mmCIF) formats.

A succinct proof of the spherical law of cosines, *i.e.* equation (2), is given by **F. C. Phillips** in ***An Introduction to Crystallography*, 4th edition, Oliver & Boyd, Edinburgh (1971) *p.* 196** and it is moderately useful since all the other laws can be derived from this one.

I am very grateful to Dr Ian Tickle (Global Phasing Ltd, Cambridge, UK) for commenting on this manuscript.

Please send any further comments, corrections and suggestions to the author so I can correct any errors or omissions (e-mail: jbcooper@fastmail.net).

- Written with **Gummi** - the simple LaTeX editor -