Frac-to-cart-coordinates implementation aspects

Coordinate transformation in crystallography

In crystallography, atomic positions within a crystal's unit cell can be described using:

- **Fractional coordinates** $(x/a, y/b, z/c)$, which refer to the natural axes a, b, c, scaled by their respective unit cell lengths.
- **Orthogonal coordinates** (X, Y, Z), which use a right-angled Cartesian system with distances measured in Ångstroms.

For triclinic unit cells, the relationship between these coordinate systems involves a transformation matrix with non-trivial elements.

Transformation matrix

This implementation follows the methodology described on Jon Cooper's website.[1] It relies on the fundamental principles of spherical trigonometry, allowing the cosine rule for reciprocal angles:

$$\cos(\alpha^*) = \frac{\cos(\beta)\cos(\gamma) - \cos(\alpha)}{\sin(\beta)\sin(\gamma)}. \tag{1}$$

Using this, the transformation matrix to convert Cartesian orthogonal coordinates (X, Y, Z) to fractional ones (x, y, z) aligning a with the X-axis, is:

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} a & b\cos(\gamma) & c\cos(\beta) \\ 0 & b\sin(\gamma) & -c\sin(\beta)\cos(\alpha^*) \\ 0 & 0 & c\sin(\beta)\sin(\alpha^*) \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{2}$$

where a, b, c are the unit cell lengths, α, β, γ are the angles of the unit cell (in radians), and α^* is the reciprocal angle, calculated using the cosine rule above.

References

[1] Cooper, J. Very Simple Crystallographic Coordinate Transformation Tool, can be found under https://ic50.org/fractorth/.