3.3. Molecular modelling and graphics

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3.3.1. Graphics

3.3.1.1. *Coordinate systems, notation and standards*

3.3.1.1.1. *Cartesian and crystallographic coordinates*

It is usual, for purposes of molecular modelling and of computer graphics, to adopt a Cartesian coordinate system using mutually perpendicular axes in a right-handed system using the ångström unit or the nanometre as the unit of distance along such axes, and largely to ignore the existence of crystallographic coordinates expressed as fractions of unit-cell edges. Transformations between the two are thus associated, usually, with the input and output stages of any software concerned with modelling and graphics, and it will be assumed after this section that all coordinates are Cartesian using the chosen unit of distance as the unit of coordinates. For a discussion of coordinate transformations and rotations without making this assumption see Chapter 1.1 in which formulations using co- and contravariant forms are presented.

The relationship between these systems may be written

$$\mathbf{X} = \boldsymbol{M}\mathbf{x} \quad \mathbf{x} = \boldsymbol{M}^{-1}\mathbf{X}$$

in which $\mathbf{X}$ and $\mathbf{x}$ are position vectors in direct space, written as column vectors, with $\mathbf{x}$ expressed in crystallographic fractional coordinates (dimensionless) and $\mathbf{X}$ in Cartesian coordinates (dimension of length).

There are two forms of $\boldsymbol{M}$ in common use. The first of these sets the first component of $\mathbf{X}$ parallel to $\mathbf{a}^*$ and the third parallel to $\mathbf{c}$ and is

$$\boldsymbol{M} = \begin{pmatrix} a\varphi/\sin\alpha & 0 & 0 \\ a(\cos\gamma - \cos\alpha\cos\beta)/\sin\alpha & b\sin\alpha & 0 \\ a\cos\beta & b\cos\alpha & c \end{pmatrix}$$

$$\boldsymbol{M}^{-1} = \begin{pmatrix} \sin\alpha/a\varphi & 0 & 0 \\ (\cos\alpha\cos\beta - \cos\gamma)/b\varphi\sin\alpha & 1/b\sin\alpha & 0 \\ (\cos\alpha\cos\gamma - \cos\beta)/c\varphi\sin\alpha & -1/c\tan\alpha & 1/c \end{pmatrix}$$

in which

$$\begin{aligned}\varphi &= \sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma} \\ &= \sin\alpha\sin\beta\sin\gamma^*.\end{aligned}$$

φ is equal to the volume of the unit cell divided by abc, and is unchanged by cyclic permutation of α, β and γ and of α^*, β^* and γ^*. The Cartesian and crystallographic axes have the same chirality if the positive square root is taken.

The second form sets the first component of $\mathbf{X}$ parallel to $\mathbf{a}$ and the third component of $\mathbf{X}$ parallel to $\mathbf{c}^*$ and is

$$\boldsymbol{M} = \begin{pmatrix} a & b\cos\gamma & c\cos\beta \\ 0 & b\sin\gamma & c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma \\ 0 & 0 & c\varphi/\sin\gamma \end{pmatrix}$$

$$\boldsymbol{M}^{-1} = \begin{pmatrix} 1/a & -1/a\tan\gamma & (\cos\alpha\cos\gamma - \cos\beta)/a\varphi\sin\gamma \\ 0 & 1/b\sin\gamma & (\cos\beta\cos\gamma - \cos\alpha)/b\varphi\sin\gamma \\ 0 & 0 & \sin\gamma/c\varphi \end{pmatrix}.$$

A third form, suitable only for rhombohedral cells, is

$$\boldsymbol{M} = \frac{a}{3}\begin{pmatrix} p+2q & p-q & p-q \\ p-q & p+2q & p-q \\ p-q & p-q & p+2q \end{pmatrix}$$

$$\boldsymbol{M}^{-1} = \frac{1}{3a}\begin{pmatrix} \frac{1}{p}+\frac{2}{q} & \frac{1}{p}-\frac{1}{q} & \frac{1}{p}-\frac{1}{q} \\ \frac{1}{p}-\frac{1}{q} & \frac{1}{p}+\frac{2}{q} & \frac{1}{p}-\frac{1}{q} \\ \frac{1}{p}-\frac{1}{q} & \frac{1}{p}-\frac{1}{q} & \frac{1}{p}+\frac{2}{q} \end{pmatrix}$$

in which

$$p = \pm\sqrt{1 + 2\cos\alpha} \quad q = \pm\sqrt{1 - \cos\alpha},$$

which preserves the equivalence of axes. Here the chiralities of the Cartesian and crystallographic axes are the same if p is chosen positive, and different otherwise, and the two sets of axes coincide in projection along the triad if q is chosen positive and are π out of phase otherwise.

3.3.1.1.2. *Homogeneous coordinates*

Homogeneous coordinates have found wide application in computer graphics. For some equipment their use is essential, and they are of value analytically even if the available hardware does not require their use.

Homogeneous coordinates employ four quantities, X, Y, Z and W, to define the position of a point, rather than three. The fourth coordinate has a scaling function so that it is the quantity X/W (as delivered to the display hardware) which controls the left–right positioning of the point within the picture. A point with $|X/W| < 1$ is in the picture, normally, and those with $|X/W| > 1$ are outside it, but see Section 3.3.1.3.5.

There are many reasons why homogeneous coordinates may be adopted, among them the following:

(i) X, Y, Z and W may be held as integers, thus enabling fast arithmetic whilst offering much of the flexibility of floating-point working. A single W value may be common to a whole array of X, Y, Z values.

(ii) Perspective transformations can be implemented without the need for any division. Only high-speed matrix multiplication using integer arithmetic is necessary, provided only that the drawing hardware can provide displacements proportional to the ratio of two signals, X and W or Y and W. Rotation, translation, scaling and the application of perspective are all affected by operations of the same form, namely multiplication of a four-vector by a 4×4 matrix. The hardware may thus be kept relatively simple since only one type of operation needs to be provided for.

(iii) Since kX, kY, kZ, kW represents the same point as X, Y, Z, W, the hardware may be arranged to maximize resolution without risk of integer overflow.

For analytical purposes it is convenient to regard homogeneous transformations in terms of partitioned matrices

$$\begin{pmatrix} \boldsymbol{M} & \mathbf{V} \\ \mathbf{U} & N \end{pmatrix}\begin{pmatrix} \mathbf{X} \\ W \end{pmatrix},$$

where $\boldsymbol{M}$ is a 3×3 matrix, $\mathbf{V}$ and $\mathbf{X}$ are three-element column vectors, $\mathbf{U}$ is a three-element row vector and N and W are scalars.

Matrices and vectors which are equivalent under the considerations of (iii) above will be related by the sign $\simeq$ in what follows.

references