13.2. Rotation functions

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13.2.1. Overview

We will discuss a technique to find either the relative orientations of homologous but independent subunits connected by noncrystallographic symmetry (NCS) elements or the absolute orientations of these subunits if the structure of a similar molecule or fragment is available. The procedure makes intensive use of properties of the rotation group, so we will start by recalling some properties of rotations. More advanced results are included in Appendix 13.2.1.

13.2.2. Rotations in three-dimensional Euclidean space

A rotation **R** is specified by an oriented axis, characterized by the unit vector **u**, and the spin, χ, about it. Positive spins are defined by the right-hand screw sense and values are given in degrees. An almost one-to-one correspondence between rotations and parameters (χ, **u**) can be established. If we restrict the spin values to the positive interval $0 \le \chi \le 180$, then for each rotation there is a unique vector $\chi\mathbf{u}$ within the sphere of radius 180. However, vectors situated at opposite points on the surface correspond to the same rotation, *e.g.* (180, **u**) and (180, $-$**u**).

When the unit vector **u** is specified by the colatitude ω and the longitude φ with respect to an orthonormal reference frame (see Fig. 13.2.2.1*a*), we have the spherical polar parameterization of rotations (χ, ω, φ). The range of variation of the parameters is

$$0 \le \chi \le 180;\ 0 \le \omega \le 180;\ 0 \le \varphi < 360.$$

Rotations may also be parameterized with the Euler angles (α, β, γ) associated with an orthonormal frame (**x**, **y**, **z**). Several conventions exist for the names of angles and definitions of the axes involved in this parameterization. We will follow the convention by which (α, β, γ) denotes a rotation of α about the z axis, followed by a rotation of β about the nodal line n, the rotated y axis, and finally a rotation of γ about **p**, the rotated z axis (see Fig. 13.2.2.1*b*):

$$\mathbf{R}(\alpha, \beta, \gamma) = \mathbf{R}(\gamma, \mathbf{p})\mathbf{R}(\beta, \mathbf{n})\mathbf{R}(\alpha, \mathbf{z}). \qquad (13.2.2.1)$$

The same rotation may be written in terms of rotations around the fixed orthonormal axes. By using the group property

$$\mathbf{T}\mathbf{R}(\chi, \mathbf{u})\mathbf{T}^{-1} = \mathbf{R}(\chi, \mathbf{T}\mathbf{u}), \qquad (13.2.2.2)$$

which is valid for any rotation **T**, we obtain (see Appendix 13.2.1)

$$\mathbf{R}(\alpha, \beta, \gamma) = \mathbf{R}(\alpha, \mathbf{z})\mathbf{R}(\beta, \mathbf{y})\mathbf{R}(\gamma, \mathbf{z}). \qquad (13.2.2.3)$$

The parameters (α, β, γ) take values within the parallelepiped

$$0 \le \alpha < 360;\ 0 \le \beta \le 180;\ 0 \le \gamma < 360.$$

Here again, different values of the parameters may correspond to the same rotation, *e.g.* (α, 180, γ) and $(\alpha - \gamma, 180, 0)$.

Although rotations are abstract objects, there is a one-to-one correspondence with the orthogonal matrices in three-dimensional space. In the following sections, **R** will denote a 3×3 orthogonal matrix. An explicit expression for the matrix which corresponds to the rotation (χ, **u**) is

$$\begin{bmatrix} \cos\chi + u_1u_1(1-\cos\chi) & u_1u_2(1-\cos\chi) - u_3\sin\chi & u_1u_3(1-\cos\chi) + u_2\sin\chi \\ u_2u_1(1-\cos\chi) + u_3\sin\chi & \cos\chi + u_2u_2(1-\cos\chi) & u_2u_3(1-\cos\chi) - u_1\sin\chi \\ u_3u_1(1-\cos\chi) - u_2\sin\chi & u_3u_2(1-\cos\chi) + u_1\sin\chi & \cos\chi + u_3u_3(1-\cos\chi) \end{bmatrix} \qquad (13.2.2.4)$$

or, in condensed form,

$$\mathbf{R}(\chi, \mathbf{u})_{ij} = \delta_{ij}\cos\chi + u_iu_j(1-\cos\chi) + \sum_{k=1}^{3}\varepsilon_{ikj}u_k\sin\chi, \qquad (13.2.2.5)$$

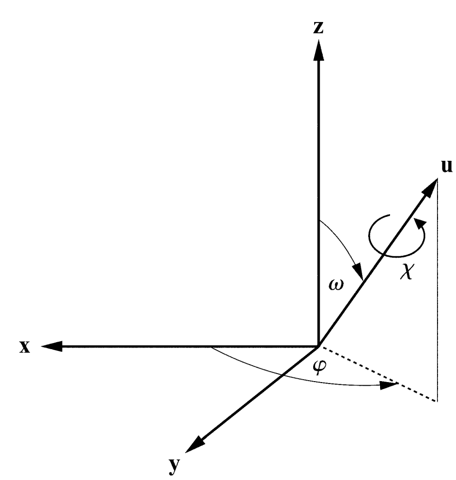
where δ_{ij} is the Kronecker tensor, u_i are the components of **u**, and ε_{ijk} is the Levi–Civita tensor. The rotation matrix in the Euler parameterization is obtained by substituting the matrices in the right-hand side of equation (13.2.2.3) by the corresponding expressions given by equation (13.2.2.4).

13.2.2.1. *The metric of the rotation group*

The idea of distance between rotations is necessary for a correct formulation of the problem of sampling and for plotting functions of rotations (Burdina, 1971; Lattman, 1972). It can be demonstrated that the quantity

$$ds^2 = \mathrm{Tr}(d\mathbf{R}\, d\mathbf{R}^{+}) = \sum_{i,j=1}^{3}(dR_{ij})^2 \qquad (13.2.2.6)$$

defines a metric on the rotation group, unique up to a multiplicative



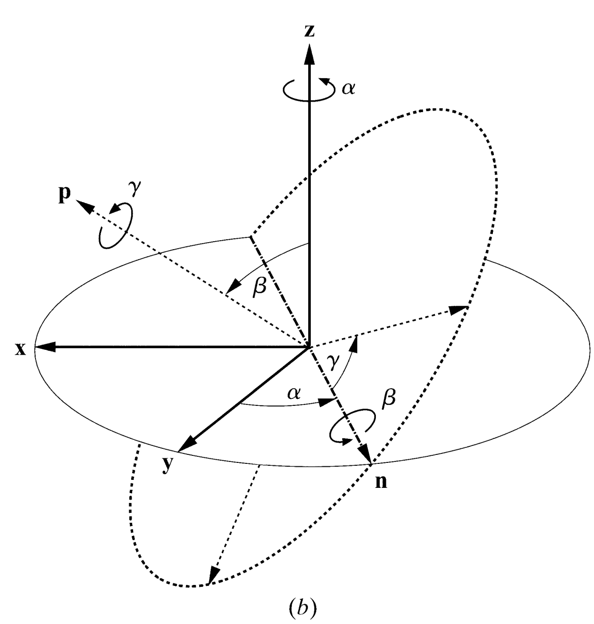


Fig. 13.2.2.1. Illustration of rotations defined by (*a*) the spherical polar angles (χ, ω, φ); (*b*) the Euler angles (α, β, γ).

references