3.1.8.2. Scalar product of vector products

$$(\mathbf{u}\wedge\mathbf{v})\cdot(\mathbf{w}\wedge\mathbf{z}) = (\mathbf{u}\cdot\mathbf{w})(\mathbf{v}\cdot\mathbf{z}) - (\mathbf{u}\cdot\mathbf{z})(\mathbf{v}\cdot\mathbf{w}). \quad (3.1.8.3)$$

A derivation of this result may be found also in Shmueli (1974).

3.1.8.3. Vector product of vector products

$$(\mathbf{u}\wedge\mathbf{v})\wedge(\mathbf{w}\wedge\mathbf{z}) = (\mathbf{u}\cdot\mathbf{w}\wedge\mathbf{z})\mathbf{v} - (\mathbf{v}\cdot\mathbf{w}\wedge\mathbf{z})\mathbf{u} \quad (3.1.8.4)$$

$$(\mathbf{u}\wedge\mathbf{v})\wedge(\mathbf{w}\wedge\mathbf{z}) = (\mathbf{u}\cdot\mathbf{v}\wedge\mathbf{z})\mathbf{w} - (\mathbf{u}\cdot\mathbf{v}\wedge\mathbf{w})\mathbf{z}. \quad (3.1.8.5)$$

3.1.9. Planes

Among several ways of characterizing a plane in a general rectilinear coordinate system is a description in terms of the coordinates of three non-collinear points that lie in the plane. If the points are U, V and W, lying at the ends of vectors **u**, **v** and **w**, the vectors $\mathbf{u}-\mathbf{v}$, $\mathbf{v}-\mathbf{w}$ and $\mathbf{w}-\mathbf{u}$ are in the plane. The vector

$$\mathbf{z} = (\mathbf{u}-\mathbf{v})\wedge(\mathbf{v}-\mathbf{w}) \quad (3.1.9.1)$$

is normal to the plane. Expansion of (3.1.9.1) yields

$$\mathbf{z} = (\mathbf{u}\wedge\mathbf{v}) + (\mathbf{v}\wedge\mathbf{w}) + (\mathbf{w}\wedge\mathbf{u}). \quad (3.1.9.2)$$

Making use of (3.1.7.1),

$$\mathbf{z} = \varepsilon_{ijk}(u^j v^k + v^j w^k + w^j u^k)\mathbf{a}^i. \quad (3.1.9.3)$$

If now **x** is any vector from the origin to the plane, $\mathbf{x}-\mathbf{u}$ is in the plane, and

$$(\mathbf{x}-\mathbf{u})\cdot\mathbf{z} = 0. \quad (3.1.9.4)$$

From (3.1.9.2),

$$\mathbf{u}\cdot\mathbf{z} = \mathbf{u}\cdot\mathbf{v}\wedge\mathbf{w}. \quad (3.1.9.5)$$

Rearrangement of (3.1.9.4) with $\mathbf{x}\cdot\mathbf{z}$ on the left and $\mathbf{u}\cdot\mathbf{z}$ on the right, and using (3.1.9.3) for **z** on the left leads to

$$\varepsilon_{ijk}x^i(u^j v^k + v^j w^k + w^j u^k) = \varepsilon_{ijk}u^i v^j w^k. \quad (3.1.9.6)$$

If, in particular, the points are on the coordinate axes, their designations are $[u^1, 0, 0]$, $[0, v^2, 0]$ and $[0, 0, w^3]$, and (3.1.9.6) becomes

$$x^1/u^1 + x^2/v^2 + x^3/w^3 = 1, \quad (3.1.9.7)$$

which may be written

$$x^i h_i = 1 \quad (3.1.9.8)$$

or

$$\mathbf{x}\cdot\mathbf{h} = 1 \quad (3.1.9.9)$$

in which the vector **h** has coordinates

$$\mathbf{h} = (1/u^1, 1/v^2, 1/w^3). \quad (3.1.9.10)$$

That is, the covariant components of **h** are given by the reciprocals of the intercepts of the plane on the axes. The vector **h** is normal to the plane it describes (Sands, 1982*a*) and the length of **h** is the reciprocal of the distance d of the plane from the origin; *i.e.*,

$$h = 1/d. \quad (3.1.9.11)$$

If the indices h_i are relatively prime integers, the theory of numbers tells us that the Diophantine equation (3.1.9.8) has solutions x^i that are integers. Points whose contravariant components are integers are lattice points, and such a plane passes through an infinite number of lattice points and is called a *lattice plane*. Thus, the h_i for lattice planes are the familiar Miller indices of crystallography.

Calculations involving planes become quite manageable when the normal vector **h** is introduced. Thus, the distance l from a point P with coordinates p^i to a plane characterized by **h** is

$$l = (1 - \mathbf{p}\cdot\mathbf{h})/h, \quad (3.1.9.12)$$

where a negative sign indicates that the point is on the opposite side of the plane from the origin.

The dihedral angle τ between planes with normals **h** and $\mathbf{h}'$ is

$$\tau = \cos^{-1}[-\mathbf{h}\cdot\mathbf{h}'/(hh')]. \quad (3.1.9.13)$$

A variation of (3.1.9.13) expresses τ in terms of vector **u** in the first plane, vector **w** in the second plane, and vector **v**, the intersection of the planes, as (Shmueli, 1974)

$$\tau = \cos^{-1}[(\mathbf{u}\wedge\mathbf{v})\cdot(\mathbf{v}\wedge\mathbf{w})/|\mathbf{u}\wedge\mathbf{v}||\mathbf{v}\wedge\mathbf{w}|]. \quad (3.1.9.14)$$

A similar calculation gives angles of torsion. Let $\mathbf{t}_h$ and $\mathbf{u}_h$ be, respectively, the projections of vectors **t** and **u** onto the plane with normal **h**.

$$\mathbf{t}_h = \mathbf{t} - (\mathbf{t}\cdot\mathbf{h})\mathbf{h}/h^2 \quad (3.1.9.15)$$

$$\mathbf{u}_h = \mathbf{u} - (\mathbf{u}\cdot\mathbf{h})\mathbf{h}/h^2. \quad (3.1.9.16)$$

The angle between $\mathbf{t}_h$ and $\mathbf{u}_h$ represents a torsion about **h** (Sands, 1982*b*). Another approach to the torsion angle, which gives equivalent results (Shmueli, 1974), is to compute the angle between $\mathbf{t}\wedge\mathbf{h}$ and $\mathbf{u}\wedge\mathbf{h}$ using (3.1.8.3).

3.1.10. Variance–covariance matrices

Refinement of a crystal structure yields both the parameters that describe the structure and estimates of the uncertainties of those parameters. Refinement by the method of least squares minimizes a weighted sum of squares of residuals. In the matrix notation of Hamilton's classic book (Hamilton, 1964), values of