The Angle between a Line and a Plane

Software now used by chemists can display a model of a crystal lattice in which it is possible by clicking on the images of atoms in the lattice to determine the distance between any two atoms and the angle $\angle ABC$ formed by the rays from the atom at B through the atom at A and the atom at C. Given this software, the problem arises of computing the angle formed by a line through two atoms at D and E with the plane of the atoms at points A, B, and C. The problem would be a simple matter of analytic geometry if one only had a coordinate system. Thus we must attempt to supply this lack from information that the software can provide. The situation is shown in the figure below. From the software we can determine the following constants:

1. The distances $AD = d$ and $AE = e$.
2. The angles $\angle ABC = \theta$, $\angle ABD = \lambda$, $\angle ACD = \mu$, $\angle ABE = \rho$, $\angle ACE = \sigma$.

We need to get coordinates for D and E in terms of a rectangular coordinate system with origin at A, positive x-axis along the ray from A through B, and xy-plane containing A, B, and C. If $D = (d_1, d_2, d_3)$ and $E = (e_1, e_1, e_3)$ in such a coordinate system, then the angle τ between the ray from D through E and the plane of A, B, and C will be

$$\tau = \arctan\left(\frac{|e_3 - d_3|}{\sqrt{(e_1 - d_1)^2 + (e_2 - d_2)^2}}\right).$$

(We use the absolute value here since orientation does not matter. We regard all angles as positive.) In order to do find these coordinates, we need to get the dihedral angle φ between the plane of ABC and the plane of ABD and the dihedral angle ψ between the plane of ABC and the plane of ABE. This is most easily done using spherical trigonometry.

Imagine a sphere of large radius with center at A, and project the points B, C, and D from the center to points B', C', D' on this sphere, thereby forming a spherical triangle. The angle at B' in this spherical triangle will be φ. The side $B'D'$ will be λ, side $B'C'$ will be θ, and $C'D'$ will be μ. By the spherical law of cosines, we have

$$\cos\mu = \cos\theta\cos\lambda + \sin\theta\sin\lambda\cos\varphi. \tag{1}$$

Similarly

$$\cos\sigma = \cos\theta\cos\rho + \sin\theta\sin\rho\cos\psi. \tag{2}$$

Equations (1) and (2) determine the dihedral angles φ and ψ in terms of angles that can be provided by the software.

The coordinates of D are now easily given:

$$D = (d\cos\lambda,\, d\sin\lambda\cos\varphi,\, d\sin\lambda\sin\varphi). \tag{3}$$

Similarly,

$$E = (e\cos\rho,\, e\sin\rho\cos\psi,\, e\sin\rho\sin\psi). \tag{4}$$

It then follows that

$$\tau = \arctan\left(\frac{|e\sin\rho\sin\psi - d\sin\lambda\sin\varphi|}{\sqrt{(e\cos\rho - d\cos\lambda)^2 + (e\sin\rho\cos\psi - d\sin\lambda\cos\varphi)^2}}\right).$$