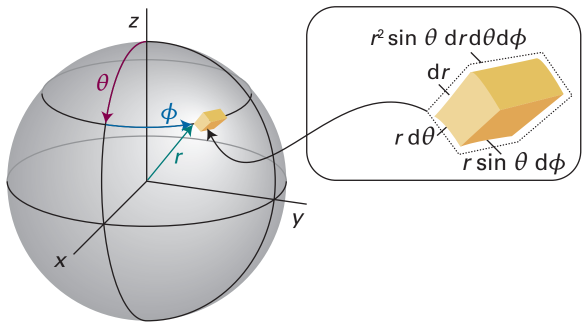
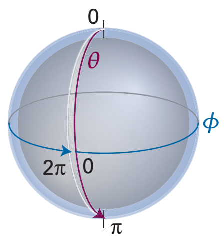
THE CHEMIST'S TOOLKIT 21 Spherical polar coordinates

The mathematics of systems with spherical symmetry (such as atoms) is often greatly simplified by using **spherical polar coordinates** (Sketch 21.1): r, the distance from the origin (the radius), θ, the colatitude, and ϕ, the azimuth. The ranges of these coordinates are (with angles in radians, Sketch 21.2):

$$0 \le r \le +\infty,\ 0 \le \theta \le \pi,\ 0 \le \phi \le 2\pi$$



Sketch 21.1



Sketch 21.2

An angle in radians is defined as the ratio of the length of an arc, s, to the radius r of a circle, so $\theta = s/r$. For a complete circle, the arc length is the circumference, $2\pi r$, so the angle subtended in radians for a complete revolution is $2\pi r/r = 2\pi$. That is, 360° corresponds to 2π radians, and consequently 180° corresponds to π radians.

Cartesian and polar coordinates are related by

$$x = r\sin\theta\cos\phi \quad y = r\sin\theta\sin\phi \quad z = r\cos\theta \tag{21.1}$$

The volume element in Cartesian coordinates is $\mathrm{d}\tau = \mathrm{d}x\mathrm{d}y\mathrm{d}z$, and in spherical polar coordinates it becomes

$$\mathrm{d}\tau = r^2\sin\theta\,\mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi \tag{21.2}$$

An integral of a function $f(r,\theta,\phi)$ over all space in polar coordinates therefore has the form

$$\int f\,\mathrm{d}\tau = \int_0^\infty\int_0^\pi\int_0^{2\pi} f(r,\theta,\phi)r^2\sin\theta\,\mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi \tag{21.3}$$

where the limits on the integrations are for r, θ, and ϕ, respectively.