Representations of Orbitals

When we attempt to represent orbitals by drawings or models, we are trying to show how the electron wave function, Ψ, or (more often) the probability for the electron, $\propto \Psi^2$, is distributed in space; i.e., where it is high, low, or zero (a node). Sometimes the representations take on the appearance of physical objects, but it is important to keep in mind that these are simply representations of mathematical quantities. Thus, when we say something like "This electron is in the 1*s* orbital.", what we really mean is that the electron behaves according to the wave function Ψ for which $n = 1$, $l = 0$, and $m_l = 0$. The following are standard ways of graphically or pictorially representing the variation of Ψ or Ψ^2 in space about the nucleus.

1. *Radial Plot*: Ψ vs. r or Ψ^2 vs. r
   This is a two-dimensional plot of Ψ or Ψ^2 versus the distance, r, from the nucleus, without trying to show the three dimensional aspects of the distribution. Sometimes a particular direction in space is chosen (x, y, z) instead of any direction r.

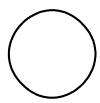
2. *Radial Distribution Function*: $4\pi r^2\Psi^2$ vs. r
   This shows the probability of finding the electron within a vanishingly thin spherical shell with a radius of r from the nucleus. Going out from the nucleus, this shows the variation in probability on the surface of increasingly larger spherical shells.

3. *Electron Charge Cloud (Electron Density) Diagram*
   This is a three-dimensional picture of Ψ^2 in which higher probability is rendered by darker shading or stippling. Most of such diagrams are meant to show approximately 90-99% of the total probability.

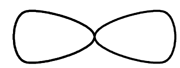
4. *Contour Diagram*
   This is a two-dimensional cross section (slice) through the probability distribution. Lines on the drawing connect regions of equal probability, much like isobars on a weather map connect regions of equal pressure.

5. *Boundary Surface Diagram*
   This is a three-dimensional solid model (or a picture of such a model) constructed so as to represent a surface that encloses approximately 90-99% of the total probability. These are sometimes called "balloon models". Sketches of orbitals used in routine work are generally two-dimensional representations of "balloon models". The usual kinds of shapes that we use in such sketches are shown on the reverse of this page.

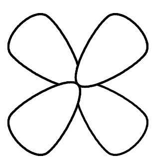
Shapes of Typical Two-Dimensional Sketches of Simple "Balloon Models"



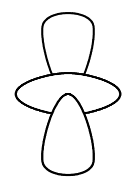
s orbital



p orbital



d orbital
(d_{xy}, d_{yz}, d_{xz}, or $d_{x^2-y^2}$)



d_{z^2} orbital

When showing specific p or d orbitals, the drawing *must* be oriented properly relative to appropriate axes. In the case of p orbitals, p_x lies along the x axis, p_y lies along the y axis, and p_z lies along the z axis. In the case of d orbitals of the "cloverleaf" type, the d_{xy}, d_{yz}, and d_{xz} orbitals lie in the plane named in their subscript, with their lobes *between* the named axes. The other "cloverleaf" type orbital, $d_{x^2-y^2}$, lies in the xy plane like the d_{xy} orbital, but its lobes are *on* the named axes. The d_{z^2} orbital has the unique "dumbbell-and-doughnut" shape shown above. The lobes of the "dumbbell" lie along z, and the "doughnut" lies in the xy plane.