NAME ___________________________________ Conference Section ________________________________

CHEM 101 CONFERENCE **Star Module – Exploration 4C**
SEPTEMBER 12/13, 2007

Wavefunctions in Three Dimensions

The three-dimensional wavefunctions, ψ, for an electron in an atom are also referred to as **atomic orbitals**. It is easier to visualize atomic orbitals by plotting electron probability density, ψ^2. In this activity, you will use the molecular modeling software *Spartan* to explore the shapes of atomic orbitals. An additional handout is available that explains how to work with *Spartan*.

In *Spartan*, open up the "surface" and "slice" corresponding to the 2*p* orbital.

1. Sketch the characteristic shape of a 2*p* orbital. Use the "slice" to probe the electron density within the mesh boundary surface of the orbital. Indicate in your drawing, the regions where a 2*p* electron is most likely to be found.

Nodes occur in atomic orbitals just as in the example of the wavefunctions of a vibrating guitar string. A node is defined to be where the wavefunction amplitude equals zero. When a node is crossed, the wavefunction amplitude changes sign. In *Spartan*, the sign of the amplitude is denoted with different colors (either red or blue).

2. (a) Orbitals represent the probability of finding an electron in a particular region of space. What is the probability of finding an electron at a node?

   (b) Nodes in orbitals come in two types that have different shapes: *radial nodes* are spherical surfaces and *angular nodes* are most typically planes. Regardless of the type, the wave amplitude is zero everywhere on the nodal surface. There is one node in the 2*p* orbital. Is this a radial node or an angular node?

   Draw in the location of the node (use a dashed line) on your picture in question 1.

In an atom, the *p* orbitals in a given shell (labeled with *n*, the principal quantum number) come in sets of 3. Open up all 3 "surfaces" representing the three different 2*p* orbitals at the same time. Try using *Mesh*, *Solid*, and *Transparent* "Styles" to distinguish the orbitals. Close any "slices" to simplify what you are looking at.

3. (a) Draw these three 2*p* orbitals on the same atom using a set of Cartesian axes to aid in representing spatial orientations. (Different colors for each orbital might be helpful.)

(b) Do the 3 different 2*p* orbitals all have the same energy? Explain.

Now close the 2*p* orbitals and open up the 2*s* orbital (both the “surface” and the “slice”).

4. (a) Sketch the characteristic shape of a 2*s* orbital. Indicate on your drawing the regions where you are most likely to find the electron, and the locations of any nodes.

(b) How many nodes are there in the 2*s* orbital? Are these spherical surfaces or planes?

Compare the 1*s*, 2*s*, and 3*s* orbitals by looking at the surface and slice for each orbital.

5. (a) What is similar about the 1*s*, 2*s*, and 3*s* orbitals?

(b) How do the sizes of the orbitals vary with *n*, the principal quantum number?

(c) Count the number of nodes in each of these orbitals. How does the number of nodes in an orbital compare to *n*, the principal quantum number? To check whether your answer is generally applicable, compare the nodes in the 2*p* and the 3*p* orbitals using *Spartan*.

(d) According to Coulomb's Law, which electron, 1*s*, 2*s*, or 3*s*, will require the *least* energy to be removed from the atom. Explain.

(e) Represent the energies of the 1*s*, 2*s*, and 3*s* orbitals on an energy level diagram. Which of these orbitals has the highest energy? The lowest energy? Justify your answer.

Open up one of the 3*d* orbitals.

6. (a) Sketch the characteristic shape of a 3*d* orbital. Indicate on your drawing the regions where you are most likely to find the electron, and the locations of any nodes.

b) On a given atom, *d* orbitals with the same principal quantum number come in sets of how many? How do you know? *Note:* Not all of the 3*d* orbitals are available to look at for the fluoride anion.