Assignment 9

Due Wednesday, November 10, 2010

Topics: This week we will finish looking at different representations of the hydrogen atom wavefunctions to help us better understand their structure and their role in determining the chemistry of atoms. This will form the groundwork for our exploration of multielectron atoms, periodic properties, and chemical bonding throughout the remainder of the semester. To date, we have discussed only one electron systems because they are by far the simplest. Apart from the hydrogen atom, we rarely encounter one electron systems in the real world, however. We need to understand how the structures of multielectron atoms differ from that of hydrogen. To do so, we must determine how to extend our conception of orbitals to multielectron systems. We will first discuss the concept of electron spin, which is the last of the four quantized values of electrons. Spin determines how electrons occupy orbitals and leads to the Pauli exclusion principle. Together with the Aufbau principle and Hund's rule, we can use the Pauli principle to determine the ground state electron configurations of multielectron atoms. These electronic arrangements give rise to the structure of the periodic table, and they provide clues to many properties of atoms, including atomic size and orbital energies.

Reading & Problems: Zumdahl, 6^{th} edition

Date	Lecture	Reading	Problems
Wednesday, 11/3	H- atom & orbitals	Section 12.8-12.9	Chapter 12: # 60, 62
Friday, 11/5	Polyelectronic atoms	Section 12.10-12.12	Chapter 12: # 65
Monday, 11/8	Aufbau principle & Periodic Table	Sections 12.13	Chapter 12: #66,70,78,80
Wednesday, 11/10	Periodic Trends	Sections 12.14-12.15	

Additional problems:

A1. On a single graph, draw the radial probability distribution $4\pi r^2(R(r)^2)$ of each possible orbital with $n = 4$. Be sure to label each distribution function.

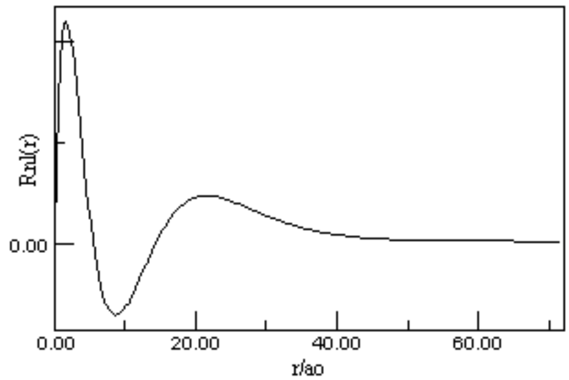
A2. On a single graph, draw the radial probability distribution $4\pi r^2(R(r)^2)$ of each possible s orbital ($l = 0$) with $n = 1$ to 4. Be sure to label each distribution function.

Note on A1 and A2: You can use the quantum numbers to determine the number of radial nodes for each case. You do not need to find the exact locations of the radial nodes – it is sufficient that the functions you sketch have the correct number of radial nodes.

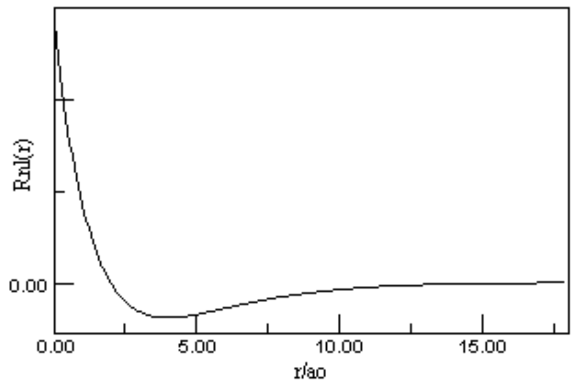
Challenge problem:

1a. Shown below are plots of the radial portion of the wavefunction vs. r. In all cases, the principle quantum number is between 2 and 4. In each case, identify the orbital, the number and type of nodes, and give one possible set of four quantum numbers for an electron in the orbital. Additionally, indicate on the plots the phase(s) of the wavefunction and the positions (and types) of the nodes. Make sure you examine the x-axis.

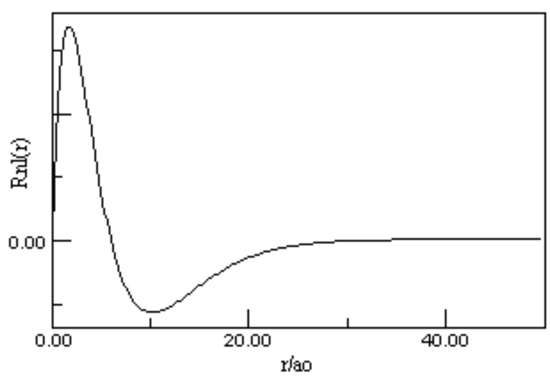
#1



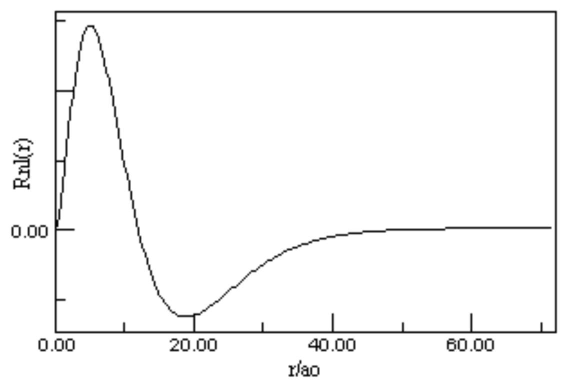
#2



#3



#4



1b. For orbitals #1 and #2 in part a, draw qualitative plots of the radial portion of the wave function squared (probability density) and the radial probability distribution vs. r. Indicate what orbital you are plotting, the radial nodes, and the most probable distances. Be sure to label both axes.

1c. The figure below shows a slice through the yz plane for some of the orbitals that have a principle quantum number of 3. Based on what you know about these orbitals, list all orbitals (with a principle quantum number of 3) that this figure applies for. In case you were wondering, nothing is wrong with the picture, it truly is completely blank.