CHEM455A - Homework 6 -- Due Mon. Nov 6 at 5PM in the Professor's Mailbox Circle your answers. Submit your problems in order. *Staple your work together*.

Text Problems

9.2-Associating Eigenfunctions with Energy eigenvalues for H-atom

9.10-Check a solution to the radial equation (if you have a first printing the first R(r) is a typo)

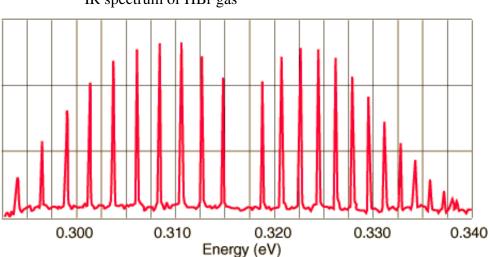
9.14-<r> as a function of Z

9.15-ionization energies for higher Z atoms. Verify that the formula in 9.15 has units of energy. 9.16-first encounter with screening

Additional Problems

1) What are the shapes of the surfaces in spherical polar coordinates where a) r is constant, b) theta is constant, c) phi is constant? Sketch them.

2) An experimental IR spectrum of HBr gas is shown below.



IR spectrum of HBr gas

a) Use the spectrum above to calculate the force constant of the bond

b) Use the spectrum above to calculate the length of the bond

c) If a similar spectrum was taken for HCl, would you expect it to be centered at HIGHER or LOWER energies. WHY?

d) How would the spectrum change as the temperature was lowered? Draw what the spectrum would look like at T=0 K.

3) What is the probability of finding an electron between r and r+dr for the hydrogen atom? Show that the *most probable* distance of finding the electron from the proton in hydrogen (in the 1s state) is a_0 , the Bohr radius. Compare this with the $\langle r \rangle$ as calculated in 9.11. Why are the two different?

4) How fast do electrons move in heavy atoms? Estimate the answer by:

a) calculating the most probable distance of finding a 1s electron from a Uranium nucleus that has been ionized of all but 1 electron

b) calculating the potential energy (U) of an electron at this distance from a U nucleus c) take this as an *estimate* of the <U> (average potential energy) of this electron. Use the virial theorem result from Example problem 9.2 to calculate <KE> for this <U>.

d) How fast would an electron with a KE equal to the <KE> you calculated have to be moving? e) Comment