Gustavus Adolphus College

CHE-372

Assignment #4

Recommended Problems (not to be handed in) All of these problems are from McQuarrie & Simon. 6-2, 6-16, 6-17, 6-46, E-8, 7-8, 7-16, 7-21, 7-22

Required Problems (Due March 28 by end of lab)

1. Prepare a hand-drawn sketch of the *X* and *B* electronic potential energy surfaces for I_2 with the corresponding vibrational energy levels. Label all of the quantities that were determined in the I_2 experiment. (This is based on your results from the I_2 lab and handout).

2. From McQuarrie & Simon: 6-25, 6-42, E-1(note: first determinant only; all others are equal to result of first), E-5, E-7, 7-9, 7-11, 7-20(a,c,e), 7-25

- 3. Use the link 'Hydrogen Atom Wavefunctions' on the course website for the following: (Note: Instead of 'sketching', you can print out each of the wavefunctions.)
 - a) Sketch the cross sections of ψ_{100} , ψ_{200} , ψ_{300} , and ψ_{900} . Comment on the general shape and the differences of the orbitals. How do we know the number of nodes in each wavefunction?
 - b) Sketch the cross sections of ψ_{210} , ψ_{211} , and ψ_{21-1} . Comment on the shapes of the orbitals.
 - c) Sketch the cross sections of ψ_{310} , ψ_{410} , and ψ_{510} . How do these wavefunctions differ from those in part b (apart from orientation)? Why?
 - d) Let n≥9 (choose one n value). What are the possible values of l and m? Look at several possible orbitals. Choose your favorite and sketch it. Comment on the orbital chosen (i.e., describe why it has this shape and orientation). Label the orbital s, p, d, f, etc.