Exam III
C441, Fall 2000

Instructions:

You may use any resource ***except*** each other, which is strictly forbidden. For maximum partial credit show **all** of your work, and clearly indicate the answer to numerical problems. Clearly label the axes and title of any graph you include, and choose appropriate ranges. Submit the problems **in numerical order**. If you have questions, please contact me and I will help you get started.

The exam is due on **Monday, Nov. 6 at the end of class. NO EXCEPTIONS!**

Good Luck!

1. Define the Born-Oppenheimer approximation in your own words.

2. Describe how the Hartee-Fock Self Consistent Field method is used to determine approximate wavefunctions and energies for multielectron atoms and molecules. Discuss and justify the approximations used in this method.

3. Hund's rule is used to determine the order with which atomic and molecular orbitals are filled. Give a definition of Hund's rule that could be used in a General Chemistry class (where they don't know about term symbols), and then extend it to include atomic and molecular term symbols. Give specific examples that illustrate how states (atomic and molecular) would be ordered.

4. Determine the possible term symbols and the order of the states for each of the following:

(a) F
(b) Si
(c) He^+
(d) N_2
(e) Cl_2
(f) S_2^+

5. Determine the relative bond strengths and bond lengths of Al_2, Cl_2, Si_2, P_2 and S_2.

6. Consider He_2 in it's ground electronic state and in an excited electronic state given by the electron configuration $(1s\sigma)^2(1s\sigma^*)^1(2s\sigma)^1$. Determine the bond order and term symbol of each. Sketch rough internuclear potential energy curves for each state. Would you expect either of these molecules to exist? Explain.

7. In class we discussed how Walsh diagrams could be used to rationalize the changes in electronic states as the bond angle of a triatomic molecule goes from linear to bent. Discuss how you would expect the bond angle of the following series of molecules to change in response to the number of valence electrons on the central atom: BeH_2, BH_2, CH_2, NH_2, H_2O.