Exam 3, Chem 311, 60 minutes, Dr. H. Guo, Nov. 14, 2008

You are allowed to bring a one page sheet containing equations and a calculator

I. Answer the following multiple choice questions (5 pts each), choose one answer only!.

1. Which of the following statements defines the Hartree approximation?
A. The wavefunction for Fermions is antisymmetric under exchange.
B. The total wavefunction for a multielectron atom can be written as a product of single electron wavefunctions.
C. Because the electronic mass is so much smaller than that of a nucleus, the electronic motion can be treated with a fixed nuclear framework.
D. Two electrons in two degenerate orbitals tend to have the same spin.
E. Electrons occupy different orbitals before they doubly occupy any one orbital.

2. Which of the following transitions are allowed for a single electron atom (you can ignore the Δm_l selection law)?
A. 1s → 2s.
B. 3d → 1s.
C. 3p → 2p.
D. 2s → 4s.
E. 2p → 1s.

3. How many degenerate orbitals does the n=4 shell of a hydrogenic atom have?
A. 4.
B. 8.
C. 12.
D. 16.
E. 32.

4. What are the quantum numbers for the $3p_z$ orbital?
A. n=3, l=1, m_l=0.
B. n=3, l=0, m_l=1.
C. n=1, l=0, m_l=1.
D. n=1, l=1, m_l=0.
E. n=0, l=3, m_l=1.

5. The carbon atoms in ethene ($H_2C=CH_2$) are
A. sp hybridized.
B. sp^2 hybridized.
C. sp^3 hybridized.
D. sp^3d^2 hybridized.
E. none of the above.

II. Solve the following simple problems

6. (10 pts) Calculate the band origin of the Lyman band (i.e., the n_1=1 to n_2=2 transition) of H atom in wavenumbers (the Rydberg constant for H is R_H = 109677 cm^{-1}).

7. (10 pts) Determine all atomic terms symbols for an electronic configuration $2s^1 2p^1$.

8. (10 pts) Construct the secular determinant for the following conjugate molecule using the Hückel approximation.

9. (10 pts) Write down the *electronic* Hamiltonian of the molecule H_3^+ under the Born-Oppenheimer approximation. Explain the Born-Oppenheimer approximation. Define the distances in a diagram.

III. Solve the following more complicated problems

10. (15 pts) Determine the location of the minimum of $\psi(r)$ for the following atomic orbital wavefunction: $\psi = N(2 - r/a_0)e^{-r/2a_0}$ where N and a_0 are constants. Sketch the wavefunction as a function of r.

11. (20 pts) Depict the molecular orbital energy level diagram for C_2 and write down its electronic configuration. Make sure to label all the MOs and AOs. Draw the shapes of the bonding σ and π molecular orbitals formed by the *p* orbitals of carbon. Use the bond order to determine the relative stability of C_2^+ and C_2^-.