Examination 2 - Chemistry 262 **November 11, 1998**

Name:_____ **Dr. Jay H. Baltisberger**

Please answer 5 of 6 questions, showing all calculations - 35 points each, 175 total.

1. Briefly explain why the hydrogen atom wavefunction solutions are not exact for a helium atom.

2. Given the term symbol ^{2}P for a sodium atom in an excited state ($1s^2 2s^2 2p^6 4p^1$), explain the meaning of the superscript 2 and the P. How many distinct types of wavefunctions would the ^{2}P term symbol allow in this case? Calculate the orbital angular momentum for this term symbol.

3. When doing a numerical calculation of the wavefunctions for a given atom, a common approach is called the Hartree-Fock (HF) self-consistent field (SCF) method. Describe how this approach is used to generate ground state wavefunctions and energies for a given atom.

4. Write the Slater determinant for the ground state wavefunction of a boron atom (B, 5 electrons). Use the notation $1s_A\alpha_A$, $2s_B\beta_B$, $3p_C\alpha_C$, etc. for the electrons labeled A through E, where α and β are the spin portion of the wavefunction for each electron. Explain how this determinant relates to the Pauli principle and anti-symmetry of the wavefunction.

5. For a hydrogen atom, calculate the radius (r_{2s}) at which the probability of finding the electron in then enclosed region is 90%. For hydrogen, Z = 1 and a = 0.5295×10^{-8} cm. For a spherical integral, $d\tau = r^2 \sin\theta \, dr \, d\theta \, d\phi$.

$$\Psi_{2s} = (1 / 4) (2 \pi)^{-1/2} (Z / a)^{3/2} (2 - Z r / a) e^{-Z r / 2 a}$$

6. Recall that when adding spin and orbital angular momenta to arrive at a total electronic angular momentum J, we use the sum J = | L + S | , | L + S – 1 |, …, | L – S |. What are possible J values for each of the following term symbols: ^{4}P, ^{3}D and ^{2}S.