**Examination 1** **October 15, 1999**

**Chemistry 362** **Dr. Jay H. Baltisberger**

**Name:** ________________________

**Please answer any 6 questions, showing all calculations - 25 points each, 150 total.**

**Single electron atom:** $E_n = -h c Z^2 R_J / n^2$ $R_J = (\mu_J/m_e) R$ $R = m_e e^4 / 8 \varepsilon^2 h^3 c$

**Particle in a box:** $\Psi_n = (2/a)^{1/2} \sin(2 \pi n x / a)$ $E = h^2 n^2 / 8 m a^2$

1. Suppose that an atom has (a) 2, (b) 4 electrons in different orbitals. What are the possible values of the total spin quantum number S? What is the multiplicity in each case?

2. Give the possible term symbols for (a) Sc [Ar] $3d^1 4s^2$, (b) B [He] $2s^2 2p^1$.

3. What is the orbital angular momentum of an electron in the orbitals (A) 1s, (b) 3s, (c) 3d? Give the numbers of angular and radial nodes in each case.

4. Calculate the mass of the deuteron given that the first line in the Lyman ($n = 1 \rightarrow 2$) series of H lies at 82 259.098 $cm^{-1}$ whereas that of D lies at 82 281.476 $cm^{-1}$. Calculate the ratio of the ionization energies of H and D.

5. Show by explicit integration that the $2p_z$, $2p_x$ and $2p_y$ orbitals are mutually orthogonal. Note that the wise student may not need to integrate over all coordinates ($r$, θ, φ) for each case…

$$\Psi_{2pz} = R_{2,1} \cos\theta \qquad \Psi_{2px} = R_{2,1} \sin\theta \cos\phi \qquad \Psi_{2py} = R_{2,1} \sin\theta \sin\phi$$

$$R_{2,1} = \frac{1}{4\sqrt{6}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \left(\frac{2Zr}{a_0}\right) e^{-\frac{2Zr}{4a_0}}$$

6. Identify the following statements as true or false:
   - A) In a three electron atom with electrons A, B & C, if electron A & B are exchanged and then A & C are exchanged, the wavefunction will be unchanged from the original wavefunction.
   - B) A transition from a $^2P$ state to a $^2P$ state is always forbidden.
   - C) A transition from a $^3S$ state to a $^3P$ state is always allowed.
   - D) There is no distance at which the probability of finding an electron in a 3s orbital is zero.
   - E) The potential energy between the two electrons in Helium may be treated as a constant energy and subtracted from the Hamiltonian to calculate the wavefunction analytically.
   - F) When an atom with a $^1S$ term symbol is placed in a magnetic field the energy remains unchanged.

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

8. Write the Slater determinant for the lowest energy excited state wavefunction of a beryllium atom (Be, 4 electrons). Use the notation $1s_A\alpha_A$, $2s_B\beta_B$, $3p_C\alpha_C$, etc. for the electrons labeled A through D, 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.

9. Calculate the minimum excitation energies of (a) the 33.0 kHz quartz crystal of a watch, (b) the bond between two O (16.00 amu each) atoms in $O_2$ for which $k = 1177$ N $m^{-1}$.

10. Calculate the commutator between d/dx and $x^2$.