Name _____
Student Number _____
Recitation Instructor _____

Chemistry 483
Practice examination 2
Fall 2008

1. (40 points) Define and/or characterize

   a. Secular Determinant

   b. Spin Angular Momentum

   c. Term Symbol

   d. Hund's Rules

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e Hartree-Fock Method

f. Electron configuration for the Oxygen atom

g. Energy levels for Be^{+2}

h. Spin-Orbit interaction

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2. (10 points) A trial function for the He atom has the form

$$\Phi(\vec{r}_1,\vec{r}_2)=\psi_{1s}(\vec{r}_1)\psi_{1s}(\vec{r}_2) \text{ where } \psi_{1s}(\vec{r})=\left(\alpha^3/\pi\right)^{1/2} e^{-\alpha r}$$

and results in the average value of the Hamiltonian

$$E(\alpha)=\alpha^2-\frac{27}{8}\alpha$$

Determine the optimal value of α and the predicted energy for this system.

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3. (15 points) Show that the most probable value of r in the1s state of H is a_0

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4. (5 points) Normalize the spin wavefunction. Show all steps.

$$\Psi(1,2) = \alpha(1)\beta(2) - \beta(1)\alpha(2)$$

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5. (10 points) The term symbols for an $\boldsymbol{np^3}$ electron configuration are ^{2}P, ^{2}D, and ^{4}S. Calculate the values of J associated with each of these term symbols. Which term represents the ground state? Whys?

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6. (10 points) Sketch the behaviour as a function of r of the 3s,3p, and 3d radial distribution functions for the Hydrogen atom. Label the sketches carefully.

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7. (10 points) Suppose we were to use a trial function of the form

$$\phi = c_1 e^{-\alpha r} + c_2 e^{-\beta r^2}$$

to carry out a variational calculation for the ground state energy of the hydrogen atom. Can you guess without doing any calculations what $c_1, c_2, \alpha,$ and $E_{\min}$ will be?