Chem 713

Final Exam study guide

The final exam is from 3:30pm to 5:30pm in GMCS-245, on Tuesday, May 18, 2010. You may use a calculator and your notes or textbook during the exam, but there may not be enough time to extensively review the material during the exam.

The final will include some short-answer questions related to the talks presented by the students. These will not deal with minute details of the talks, but you may want to refresh yourself on some of the topics. Relevant papers are posted at http://www.chemistry.sdsu.edu/courses/CHEM713/.

What follows is compiled from the previous study guides.

The following may appear on the exam:

- Calculations and algebraic manipulations involving $E_{\text{photon}} = h\nu = hc/\lambda$ or $\lambda_{\text{dB}} = h/p$. Example: Find the wavelength in m of radiation with a photon energy of $1.0 \cdot 10^{-24}$ J.

- Calculations and algebraic manipulations involving the solutions to the Bohr model of the atom, including (but not necessarily limited to) $E_n$, $r_n$, $v_n$, and $L = nh$. Example: Find the orbital radius in $a_0$ of an electron in the $n = 4$ state of $\text{He}^+$, according to the Bohr model.

- Calculations involving the energies and wavefunctions of the particle in a rectangular box of $N$ dimensions. Example: Find the zero-point energy in J of a hydrogen atom in a 1D box of length 2.0 Å.

- Calculations of transition energies $\Delta E$ for the one-electron atom or particle in a box. Example: Find the energy in $E_h$ of the $n = 3 \rightarrow 5$ transition in atomic hydrogen.

- Qualitative questions about the principles or systems that we’ve encountered so far. Example: Along which coordinates, if any, do the wavefunctions for the one-electron atom exhibit tunneling?

- Writing the wavefunction for any one-electron atomic orbital wavefunction, given the quantum numbers and table of functions. Example: Write the wavefunction for the 3p, $m_l = 1$ orbital.

- Integrals of the functions $\sin(ax)$, $\cos(ax)$, $e^{ax}$, and $x^a$; derivatives of any combination of these.

- Setting up integrals for applying the average value theorem, probability density, or orthogonality, given the normalized wavefunction. Example: Write, but do not
evaluate, the integral for finding the root mean square value of $\theta$, $\langle \theta^2 \rangle^{1/2}$, in a $2p_{m_l=0}$ atomic orbital wavefunction, given the wavefunctions listed in Table 6.2 on p. 152.

- Using Maple to evaluate one integral involving the radial wavefunctions in Table 6.1. Example: Find the probability density of 2s electron in Li$^{2+}$ at distances less than $2a/3$ (inside the radial node).

- Writing the Hamiltonian for any many-particle system, given the potential energy function. Example: Write the complete Hamiltonian for the $H_2$ molecule.

- Questions about the nature of the variational principle. Example: Write a reasonable, unnormalized variational wavefunction for the particle in a three-dimensional box, and circle the variational parameters that can be optimized.

- Qualitative questions about the principles or systems that we’ve encountered so far. Example: What is the ratio of $\langle \theta^2 \rangle^{1/2}$ for the $2p_{m_l=0}$ orbital to $\langle \theta^2 \rangle^{1/2}$ for the $3p_{m_l=0}$ orbital of the same one-electron atom?

- Integrals of the functions $\sin(ax)$, $\cos(ax)$, $e^{ax}$, and $x^a$; derivatives of any combination of these.

- Application of equations involving the harmonic oscillator approximation for molecular vibrations. Example: If the force constant for the IrN (iridium mononitride) molecule is 356 N/m, find the vibrational constant in cm$^{-1}$ for the most abundant isotopic form, and estimate the wavelength in nm of the radiation required to excite the $v = 1 \rightarrow 3$ transition.

- Questions about the nature of Hartree-Fock, density functional, and configuration interaction calculations. Example: A Hartree-Fock calculation yields a set of orbitals that we label 1s, 2s, and 3s in order of increasing energy (although these are not exactly the same as the Bohr one-electron orbitals). If the ground state HF wavefunction is $1s(1)1s(2)$, write an expression for the configuration interaction wavefunction that includes all single and double excitations. Don’t worry about the indistinguishability of the particles (in case you were tempted).

The following will NOT appear on the exam:

- Solving the equations of motion for a classical system.

- Solving any differential equations that we haven’t already solved in class.

- Solving the linear variational problem by diagonalizing the Hamiltonian matrix.

- Gaussian 03 calculations.