Study guide for the second midterm

Chemistry 341, Fall 2013
Physical Chemistry of Biochemical Systems

For the following, you should understand the concepts, know (have memorized) the key equations, understand what all the symbols mean, and be able to explain the equations in words and to appreciate their context. Please pay close attention to the *Summary* and the *Mathematics Needed* sections at the end of the chapters.

1 Chapter 11: Basics of quantum mechanics

- Bohr frequency relationship: $\Delta E = h\nu$

- de Broglie relation: $\lambda = h/p$

- Schrodinger equation: $-(\hbar^2/2m)(d^2\psi/dx^2) + V(x)\psi = E\psi$

- Harmonic oscillator: $E_n - (n + \frac{1}{2})h\nu$, where $\nu = \frac{1}{2\pi}\left(\frac{k}{\mu}\right)^{1/2}$

- Coulomb's law: $(q_1 q_2)/(4\pi\varepsilon_0 r)$

2 Chapter 12: Chemical bonding and molecular interactions

- Pauli principle: $\psi(1,2) = -\psi(2,1)$

- Molecular orbital wavefunction for H_2: $\psi(1,2) = [\psi_+(1)\psi_+(2)][\alpha(1)\beta(2) - \alpha(2)\beta(1)]$, where $\psi_+(1) = \left(\frac{1}{2}\right)^{1/2}[1s_A(1) + 1s_B(1)]$

- Basic bonding terms: hybridization, bonding and anti-bonding orbitals

- Combination of orbitals: if $\psi = c_A\psi_A + c_B\psi_B$, then one gets the following simultaneous equations:

$$(H_{AA} - ES_{AA})c_A + (H_{AB} - ES_{AB})c_B = 0$$
$$(H_{BA} - ES_{BA})c_A + (H_{BB} - ES_{BB})c_B = 0$$

- Bond stretching and bending, torsonal motion: $U(r) = k_r(r - r_{eq})^2$, $U(\theta) = k_b(\theta - \theta_{eq})^2$, $U(\phi) = (V_n/2)(1 + \cos(n\phi)$

- Lennard-Jones potential: $V = 4\varepsilon\left[(\sigma/r)^{12} - (\sigma/r)^6\right]$

- Dipole moments: $\mu = \sum_i q_i x_i$ or $\int \rho(x)x\,dx$