Key and guide to exam #2

Chemistry 342, (01:160:342), Spring 2016
Physical Chemistry of Biochemical Systems

Use the hints below to get you started on problems you had trouble with on the second exam. You should arrange to meet with me if you still don't understand how to do the problems.

Problem 3 Separate variables, putting all the terms with I on the left-hand-side, and all the terms with x on the right-hand-side. Perform a definite integration on both sides, from I_o to I_t on the left-hand side, and from 0 to ℓ on the right-hand side.

Problem 5 *(a)* Each of the three double bonds contains two π electrons; the two nitrogen atoms each have 3 σ bonds (using up 3 of their 5 valence electrons), so they each have two electrons left to contribute to the π system. Total is 10 π electrons. *(b)* Each of the six atoms in the ring, plus the two oxygen atoms, has a p_z atomic orbital than can contribute to the π molecular orbitals; hence there will be 8 π/π^* molecular orbitals. Five of these eight MO's will be filled with the 10 π electrons, and three will be unfilled. *(c)* Each oxygen atom contributes two electrons to the double bond to carbon; this leaves 4 valence electrons on each that are nonbonding. None of the other atoms has any nonbonded orbitals located on them.

Problem 6 Note (as the problem states) that the equilibrium position is when the *force* between the two particles is zero, not when the potential energy is zero. (Remember that the zero of energy is always arbitrary, so just setting the enegy to zero doesn't have any real meaning.) Use $F = -dV/dr$, plug in the expression for the Lennard=Jones $V(r)$, set this to zero and solve for r.

Problem 7 The determinant expands out to $(\alpha - E)^2 - (\beta - ES)^2 = 0$. You can expand this out and solve for E by using the quadratic equation. Simpler is to note that $(\alpha - E)^2 = (\beta - ES)^2$ implies that $(\alpha - E) = \pm(\beta - ES)$. (Don't forget the "$\pm$"!) Then the two solutions are $E_1 = (\alpha + \beta)/(1 + S)$ and $E_2 = (\alpha - \beta)/(1 - S)$. Note that having a nonzero S (which is always true for "real" bonds) means that the antibonding orbital, with energy E_2, is destabilized more than the bonding orbital, with energy E_1, is stabilized. This has important consequences for chemical bonding, but we don't have time to get to that in this class. Consider taking a course like CCB 421 (Atomic & Molecular Structure) if you want to learn more.