## Chemistry 124 Second Examination

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## October 20, 2008

The exam budgets 50 minutes, but you may have 60 minutes to finish it. Good answers can fit in the space provided.
Question values correspond to alloted time. Don't waste too much time on cheap questions.
Read each question carefully to see what it asks for (bold face is used to help highlight questions). Make sure you are answering the question, not just saying something vaguely relevant to its topic.

1. (4 min) Label the symmetric atomic orbital pairs that would give the following four profiles for overlap integral versus C -C distance

2. (4 min) Explain whether Correlation Energy should raise or lower a molecular energy calculated by the SCF procedure.
3. (2 min) Name two accurate QUANTITATIVE tools that would have been available to you, if you were a chemistry student in Yale's Sheffield Scientific School in the class of 1901.
4. (4 min) Assuming, perhaps unrealistically, that the atom-atom distances and overlap integrals are identical, explain, in terms of electron energies, which of the following bonds should be stronger. (A diagram would help.) the 1-electron bond of $\mathrm{H}_{2}^{+}$
the 3-electron bond of $\mathrm{He}_{2}{ }^{+}$
5. (4 min) Use the idea of plum-pudding orbitals to rank these three one-node MOs of the water molecule ( $\mathrm{A}, \mathrm{B}, \mathrm{C}$ ) by their relative energy (low, medium, high). Each orbital is shown in both top and side view, as is the molecular skeleton in the first row. Explain your reasoning in a very few words. (You need not give names or signs)


Side View


Low
Medium
High
?


A

6. (6 min) Use hybridization theory to explain whether the F-C-F angles of the $\cdot{ }^{\circ} \mathrm{CF}_{3}$ radical should be larger or smaller than the $\mathrm{H}-\mathrm{C}-\mathrm{H}$ angles of the $\cdot \mathrm{CH}_{3}$ radical. Describe the experiment that justifies your prediction.
7. (5 min) How was the Bürgi-Dunitz angle for attack of N on $\mathrm{C}=\mathrm{O}$ established experimentally?
8. (6 min) Use proper curved arrows to draw the 3 steps in a mechanistic scheme for conversion of $\mathrm{NH}_{3}$ to $\mathrm{NH}_{2} \mathrm{NH}_{3} \mathrm{Cl}$ by $\mathrm{Cl}_{2}$.
9. (6 min) According to "resonance" the properties of an amide are different from those expected for a molecule with simple carbonyl and amine groups. Briefly explain three different ways in which resonance influences the properties of protein polymers that contain multiple amide groups.
10. (9 min) Using all of the following four molecules SKETCH SIX (6) LOCALIZED "frontier" orbitals that would account for significant reactivity, and EXPLAIN the energy that makes each of them special. (Show orbital signs.)

## $\mathrm{Li}-\mathrm{CH}_{3}$

## $\mathrm{R}_{2} \mathrm{C}=\mathrm{N}-\mathrm{H}$

## R-O-O-R



