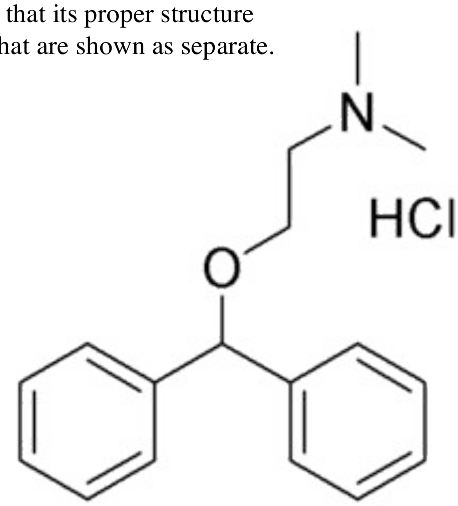
Chemistry 125 Second Examination Name ________________

October 22, 2007

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. In the last exam we encountered Benadryl (right) and considered the fact that its proper structure includes a "*pentavalent*" atom formed by reaction of the two molecules that are shown as separate.

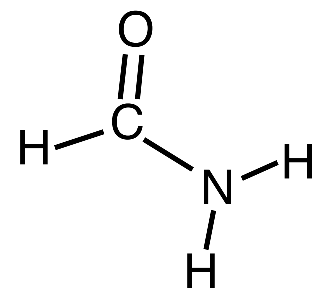


A) (2 min) Scratch out the HCl and redraw its atoms to show a proper Lewis structure for benadryl with lines for bonds.

B) (5 min) **DRAW** a reasonable representation of the **SHAPE** of the orbital that makes the **HCl** molecule reactive showing **WHERE** it should be attacked; Give a descriptive **NAME** to the molecular orbital; and **EXPLAIN** in a few words and/or with a diagram **WHY** it is reactive.

C) (4 min) **NAME TWO local orbitals** that make the **organic** (non-HCl) portion of the benadryl structure reactive. **Explain** why one should be more reactive than the other.

2. A naïve student might guess properties (total energy, HOMO/LUMO energy, reactivity, geometric structure, polarity, rigidity, *etc*.) for formamide (the molecule shown) on the basis of its possessing a carbonyl group and an amine group. A more sophisticated student (you) would point out that this molecule must be considered an "amide" with its own characteristic properties.



A) (3 min) **Explain in terms of molecular orbitals** (NOT resonance) why an amide is different in **energy** from expectations based on a "carbonyl amine".

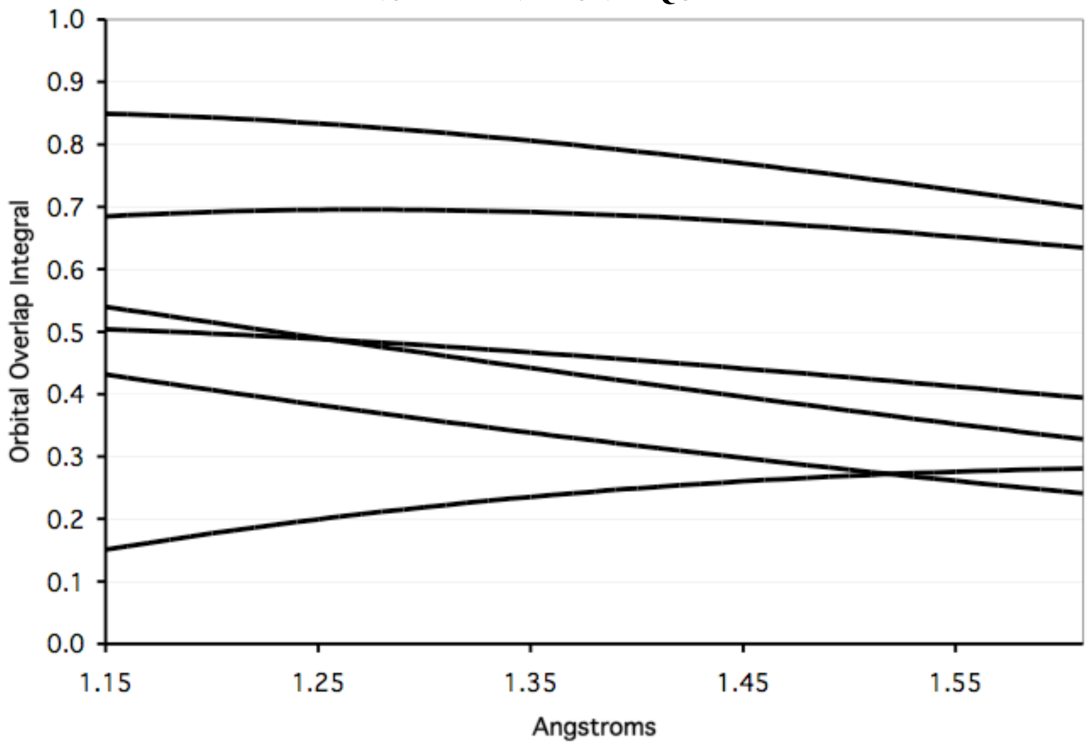
B) (4 min) **Draw** a reasonable representation of the actual **LUMO** of an amide (a few words may help explain your drawing).

C) (4.5 min) Cite **three characteristic properties of the amide group** that are important for "polypeptides" or proteins (which contain many amide groups).

3. (4.5 min) The following plot shows the **overlap integral** between valence-level atomic orbitals (**pure or hybrid**) of two carbon atoms over internuclear distances characteristic of single, double, and triple bonds.

Clearly LABEL each of the six curves with the **names of the AOs** involved (and as **sigma or pi**).

NO EXPLANATION REQUIRED

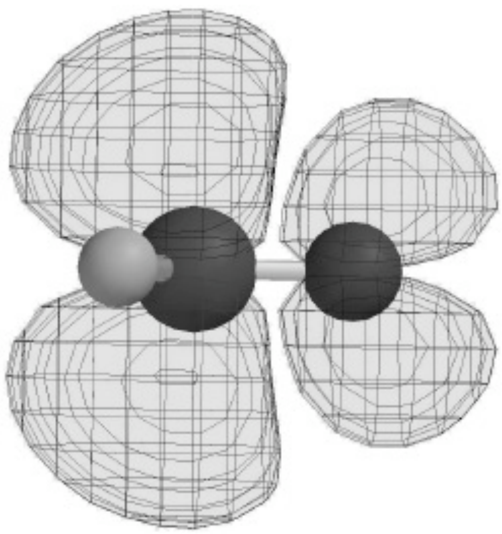


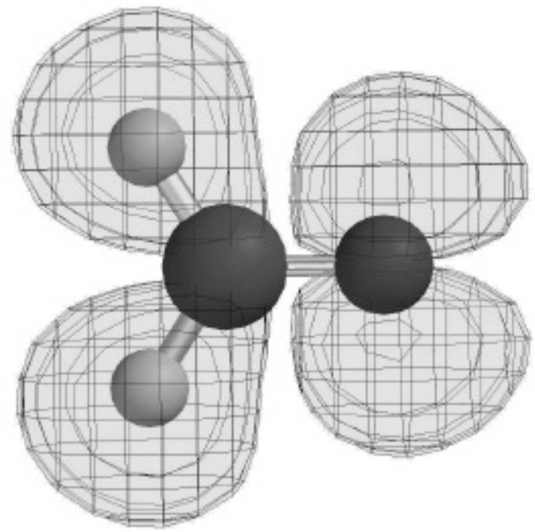
4. (4 min) **Explain** how the following question could be considered a **trick**: "Which bond is stronger H-H or H-F?"

5. (4 minutes) Here are **TWO** MOs of $H_2C{=}O$. Each has two nodes and is analogous to a *3d* atomic orbital.

A) **CIRCLE** the MO that is **LOWER** in energy, and **EXPLAIN** your choice **in terms of "plum-pudding" orbitals.**

B) In **EACH** MO draw the node that would affect the strength of a bond (one line in each picture).





6. (4 min) Why are atoms to the left of carbon in the periodic table more prone to participate in 3-center-2-electron bonds than elements to the right of carbon?

7. Trimethylamine, $(CH_3)_3N$, can be "oxidized" by hydrogen peroxide, HOOH, to give trimethylamineoxide, $(CH_3)_3NO$ in a process that involves **two reactions**.

A) (6 min) **Identify** the unusually high **HOMO** and the unusually low **LUMO** that are likely to be involved in the **first reaction** between $(CH_3)_3N$ and HOOH, **stating why** their energies are unusual.

B) (5 min) Draw the two reactions using **curved arrows** to show the electron-pair shifts involved. (Show the molecules **properly oriented** to attack one another.)