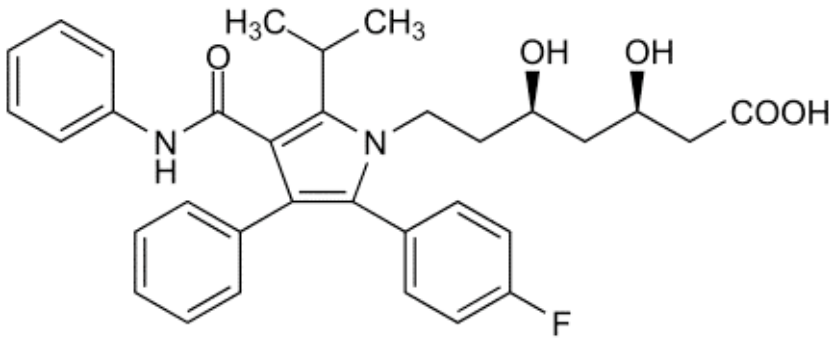
Chemistry 124 First Examination Name _____

September 25, 2009

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. (5 min) Here is atorvastatin, the active ingredient of lipitor, the world's top selling drug (> $13 billion in 2008).



Circle five **(5) DIFFERENT** functional groups in atorvastatin and **NAME THEM.**

2. (5 min) The pentagonal ring containing nitrogen in the center of atorvastatin is called pyrrole. The analogue with O for N is called furan. **Add bonds / unshared pairs / formal charges** to complete the scheme below so it shows a pair of **resonance structures** for pyrrole and a pair for furan. Use a **proper symbol** to connect the members of each pair.

Pyrrole

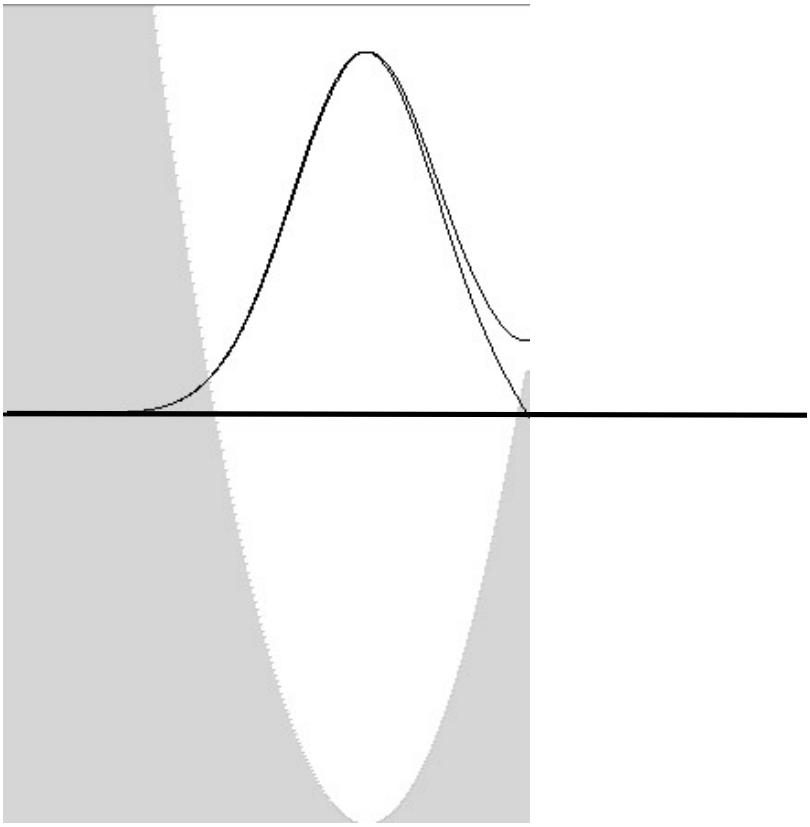
Furan

Give a reason to anticipate greater resonance stabilization in one of these molecules than in the other.

3. (4 min) **Explain briefly** how measuring the abundance of the molecular masses M, M+2, and M+4 (by mass spectroscopy) can reveal that there are two chlorine atoms in a molecule.

4. (5 minutes) Suppose your roommate understands x-ray diffraction but is a literal believer in shared-electron-pair bonds as drawn in typical Lewis dot structures. Cite a **specific experimental result** that you could use to convince your roommate to be more broadminded about the nature of bonds.

5. The diagram is ***part*** of an "Erwin Meets Goldilocks" plot with two trial wave functions for the potential energy, which is shown in gray.



A) (1.5 min) **Draw a horizontal line** showing the **TOTAL ENERGY** for ψ curve that **crosses zero** at the right.

Be as accurate as you can.

B) (1.5 min) Is the total energy for the other trial ψ (the curve that is higher at the right) **higher or lower** than that the energy you drew in A?

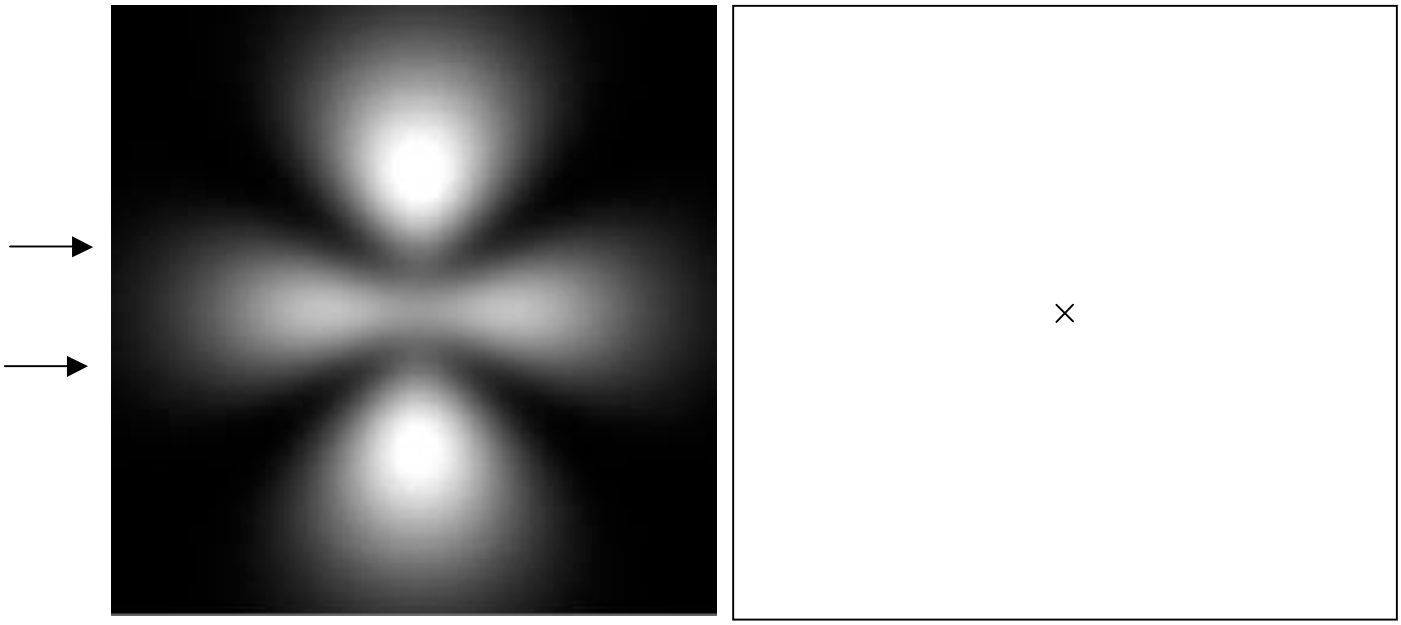
Explain your thinking.

C) (2.5 min) **Assuming** that this is a **Hooke's Law** single-minimum problem, **draw** in the **correct** lowest-energy **ψ function** (its curve, **NOT** its energy), and **extend all three ψ curves** to the right as far as possible.

D) (4.5 min) Now **assume** that this potential is in fact the left half of **a symmetric double minimum**, and the original two ψ traces are part of ***correct*** solutions. **Explain** how one ψ may be considered "bonding", and the other "antibonding".

6. The figure below displays the total 3-dimensional **electron density** of a hydrogen-like atomic orbital (from Atom-in-a Box).

(a) (3 min) In the open box sketch **several contour levels** to show the wave function (Ψ) for this orbital on a **2-dimensional SLICE** that passes through the nucleus (×), drawing **dashed line(s)** to show any node(s).



(b) (3 min) Give the **principal quantum number** for this atomic orbital: ***n* = _____**

and name the **shape of the node(s)** of the 3-dimensional orbital**: _____**

(c) (6 min) **Explain** why, in the 3-dimensional view, the **horizontal** component of the density (the part between the upper and lower arrows) appears bulbous on the ends. **In addition explain** how this answer is related to why there are two spots revealing the double helix diameter on Rosalind Franklin's x-ray photo of b-DNA.

[*Hint*: It might help to draw a picture of the same component as viewed from the top.]

7. (4 minutes) All the radial wave functions $R_{n,l}(r)$ for hydrogen-like atoms share one common mathematical function, no matter what their principal quantum numbers. **Identify this function**, and explain briefly **why** it is **reasonable** for it to be there.

8. (3 minutes) **Explain why** it is advantageous to have a scanning probe microscope with the sharpest possible tip, **AND draw a picture** the tip reported in the journal *Science* last month, **AND** give its effective **diameter** within a factor of 5.

9. (2 minutes) On the back of this page **sketch a potential energy curve** for which successive energy levels would become **MORE WIDELY spaced with increasing energy**.