## Chemistry 124 First Examination September 24, 2010

Name

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) Here is Rosiglitazone (Avandia), the diabetes drug whose withdrawal in Europe and the U.S. because of heart risks was announced yesterday (and is the headline of today's *New York Times*).



Circle four (4) DIFFERENT functional groups in Rosuvastatin and NAME THEM.

2. On the left below is shown the "thiazolidinedione" ring from Rosiglitazone.



- A. (4.5 min) Complete the three structures on the right above to show reasonable resonance structures of the ring.
- **B.** (2 min) Explain how the results of an **x-ray diffraction** study might help to decide whether the true structure of this ring in Rosiglitazone is one of the above, or whether it truly involves a resonance situation.

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**3.** (4 min) How does one go about constructing an **electron difference (or deformation) density map**. (Mention the experiments and/or theories on which it depends.)

**4.** (5 minutes) Cite **TWO different observations** from the electron difference density map of the following compound that would surprise a naïve chemist who thinks of bonds in organic molecules in terms of electron pairs shared between two nuclei.



**5.** (1 min) How much thinner than a hair was the oil slick that Benjamin Franklin measured on the pond on Clapham Common?

Circle one of the following fractions: 2/10 2/1000 2/100,000

6. (4 min) Explain which form of scanning probe microscopy yields higher resolution: STM or SNOM.

7. (1.5 min) What feature(s) of an x-ray scattering diagram characterize(s) the spacing of the repeating "unit cells"? (no explanation required)

(1.5 min) What feature(s) characterize(s) the molecular electron density distribution *within* the "unit cell"? (no explanation required)

8. (2.5 min) Since electrons behave like waves, and unlike for x-rays, there exist (electrostatic) lenses that can refocus scattered electron waves, it is possible to construct an electron microscope. In terms of quantum mechanical wave functions, explain why it is necessary to operate an electron microscopy at very high voltage (high electron kinetic energy) in order to obtain resolution of separate atoms within molecules.

- 9. All radial wave functions  $R_{n,l}(r)$  for hydrogen-like atoms share one constant factor and one mathematical function.
  - A. (3 min) Write the constant factor and the mathematical function.

**B.** (4 min) Choose **ONE** of these (the factor **OR** the function) and **explain** why it is reasonable that all  $R_{n,l}(r)$  share it.

10. Here is a one-dimensional wavefunction that solves the Schrödinger Equation for a certain particle mass and potential energy function. The dashed line shows  $\Psi = 0$ .



- A. (6 min) **Draw** over the  $\Psi$  graph above another graph showing the **POTENTIAL ENERGY** for which this  $\Psi$  is a solution. Use the **dotted line** to denote the **Total Energy**, and be as accurate and complete as you can. A few words or extra marks might help show what you are trying to draw.
- **B.** (2 min) *EXPLAIN* how many wavefunctions that solve this problem would have energies lower than this one and how many would have energies higher than this one.

C. (4 min) Describe how this wave function would change its shape as the mass of the particle is increased.