Chemistry 125 First Examination

Name _____

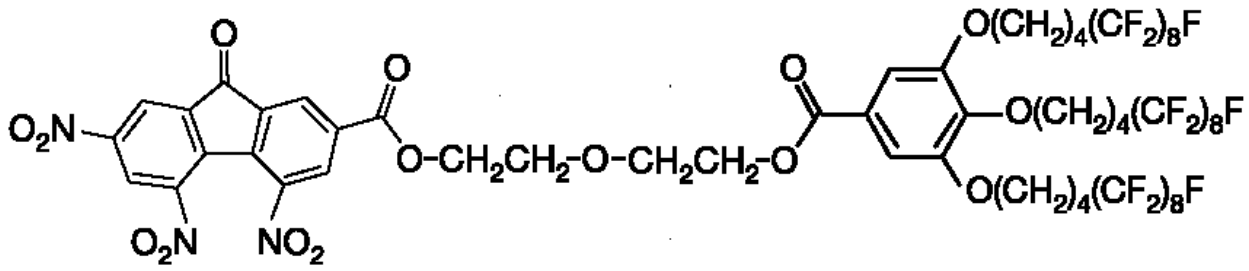
September 27, 2002

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 allotted time; don't waste too much time on cheap questions.
Read each question carefully to see what it asks for, and be sure to answer all of its parts.

1 . (4 min) **Explain** which of the following techniques would be best for measuring the distance between two copper atoms about 5Å apart on a graphite surface: AFM, STM, high-powered optical microscopy.

2. (8 min) **What is fundamentally wrong** with the idea of orbitals? How do the $\mathbf{Z_{eff}}$ and **SCF** methods attempt to circumvent this difficulty? What is "**correlation energy**"?

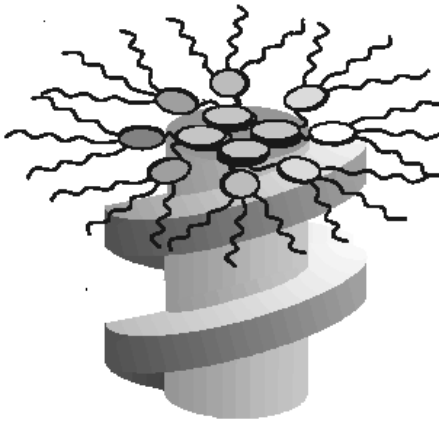
3 . (4 minutes) In yesterday's issue of the journal *Nature* [vol. 419, p. 384] is a description of "helical dendrimers" that show promise as electronic materials. The formula below shows one of the molecules discussed. **Neglecting** the three $(CH_2)_4(CF_2)_8F$ groups on the far right, **circle FOUR DIFFERENT functional groups** in this molecule and **give their names**. Make sure the groups have different names.:



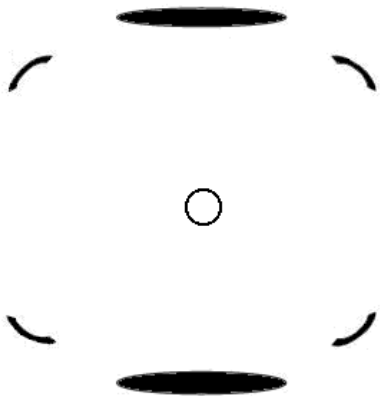
4. (6 min) The authors of the *Nature* paper suggests that molecules of the type shown in Question 3 pack together with the flat portion on the left (the part with all the NO_2s) stacked in the middle to form a cylinder and the "hairy" part on the right arranged as a helical wrapping around the cylinder, denoted by the spiral around their rough figure shown on the right

As evidence to support the stacking and the helical wrapping of this material they show a fiber's x-ray scattering pattern, six spots of which are shown below right.

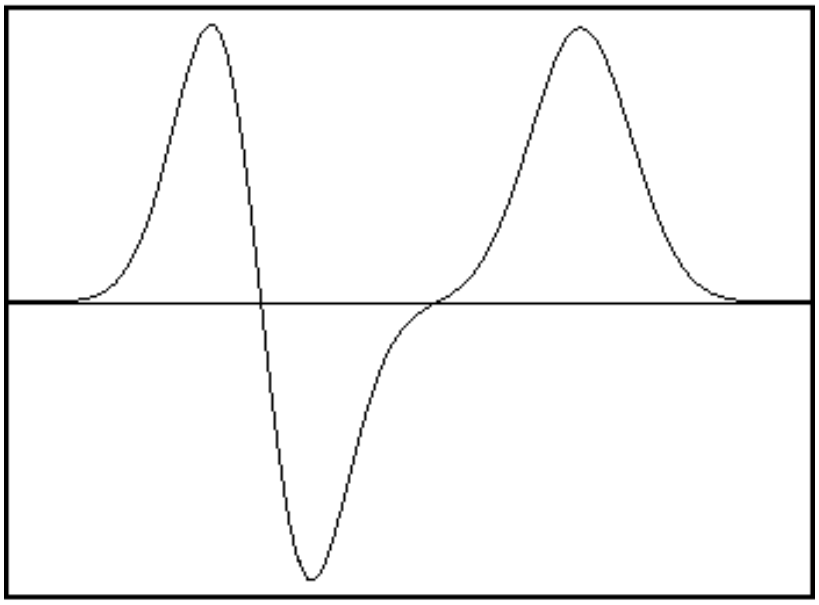
(The open circle in the middle shows where the undeflected x-ray beam would hit the film.)



Explain how the **six spots** support the existence of **stacking and helix**, and explain how the pattern shows the **spacing** of the stacking and the **pitch** (steepness) of the helix. **Is the pattern consistent** with the rough figure showing the packing?



5. (9 minutes) The top frame shows a wave function Ψ (horizontal line is at 0). Ψ is a solution to the Schrödinger equation for a particle in one dimension with a certain potential energy as a function of position and a certain total energy. In the lower frame **sketch an appropriate potential energy** for this Ψ (the central horizontal line represents the total energy). You may wish to comment and/or use lines or arrows to show correspondence in position between the wave function and the potential energy function.



6. (2 minutes) Could the wave function shown in question 5 be the lowest-energy solution for this Schrödinger equation. If not, **how many solutions of lower energy** should there be? Explain your thinking.

7 . (5 min) **What factor** appears in **all** radial wave functions [R(ρ)] for one-electron atoms? **Why** is it reasonable that they should all contain this factor?.

8 . (12 minutes) For **ONE** of the following two cases **draw** a schematic **x-ray difference density** plot, **explain** how it would be generated experimentally, **and** use it to **discuss** the curious nature of the bonding:
The C-F bond from a benzene ring **OR** The C-C bonds in a ring of three bonded carbons.

9 . (Extra Credit) As a university science student, what is the most important trait you should have in common with Joseph Nathan Kane, who died last Sunday at the age of 103? [See obituary in today's New York Times]