

Chemistry 210
“Organic Chemistry I”
Summer Semester 1999
Dr. Rainer Glaser

Examination #1

“Structure, Bonding and Properties of Organic Molecules.
Structure, Stereochemistry and Properties of Alkanes.”

Wednesday, June 23, 1999, 8:40 – 9:40

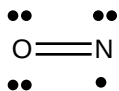
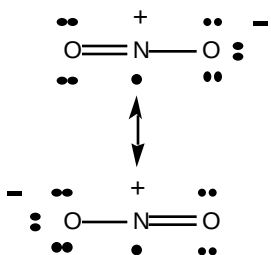
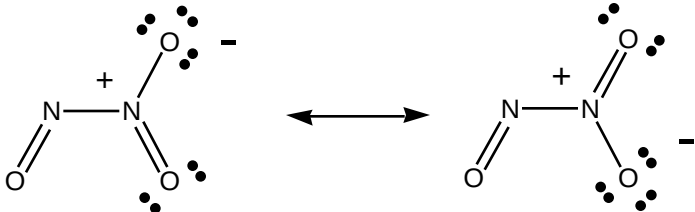
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Answer Key

Question 1. LK Structures & Hybridization. (News #1)	14	
Question 2. Organic Structures and Properties. (MC #1)	16	
Question 3. Intermol. Interactions. (News #2, VC #2)	12	
Question 4. Orbitals and Hybridization. (MC #2)	16	
Question 5. Structures and Representations of Molecules.	14	
Question 6. Alkanes. (MC #3)	16	
Question 7. Ring-flipping in Cyclohexane.	12	
Total	100	
Multiple Choice Points and Percentage:		

Question 1. Lewis-Kekule Structures & Hybridization. (14 points)

The article “U.S. FLOATS NEW 'BUBBLE' PROPOSAL” (*Asahi News Service*, December 11, 1997) brought up some timely issues in atmospheric chemistry. Nitrogenoxide, nitrogendioxide, and dinitrogen trioxide are among the molecules responsible for the greenhouse effect. Provide the Lewis-Kekule structures of the nitrogenoxides. If several resonance forms are needed for a good description of the molecule, then provide all the major resonance forms. In all cases, clearly indicate formal charges (if any).

NO  Radical? Yes - No (Circle correct)	NO₂  Radical? Yes - No (Circle correct)
ON-NO₂  Radical? Yes - No (Circle correct)	

The hybridization of the O-atom in carbondioxide:

sp²

The hybridization of the C-atom in carbondioxide:

sp

The hybridization of the N atom in HNO₃:

sp²

The overall bond order of the NO bond in NO₃⁻:

1 1/3

The π bond order of the NO bond in NO₃⁻:

1/3

Question 2. Organic Structures and Properties. (16 points)

E-Q7 What is the ground state electron configuration of sodium?

- a** $1s^2 2s^2 2p^6 3s^1$
- b. $1s^2 2s^2 2p^6 3s^2$
- c. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
- d. $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
- e. $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$

E-Q9 The ionization energy of an element “E” is the energy of which one of the following processes?

- a. $E^{2-} \rightarrow E^- + 1 e^-$
- b. $E^- \rightarrow E + 1 e^-$
- c. $E \rightarrow E^+ + 1 e^-$**
- d. $E^+ \rightarrow E^{2+} + 1 e^-$
- e. $E \rightarrow E^{2+} + 2 e^-$

E-Q17 In which one of the following bonds is the C-atom the negative pole of the bond dipole?

- a. C-H
- b. C-F
- c. C-Cl
- d. C=O
- e. C-Li**

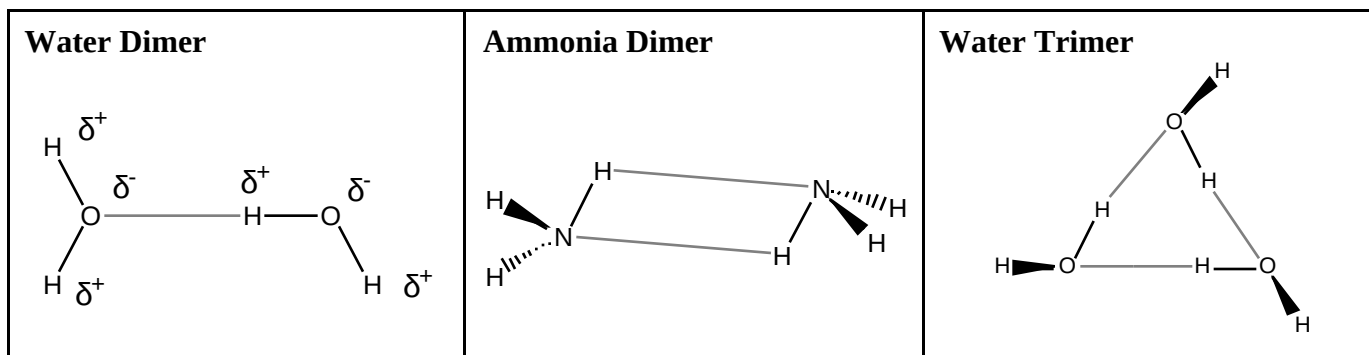
E-Q19 What are the formal charges on N and B in the complex formed between ammonia, NH_3 , and borane, BH_3 ?

- a. $FC(N) = 0$ and $FC(B) = 0$
- b. $FC(N) = +1$ and $FC(B) = -1$**
- c. $FC(N) = -1$ and $FC(B) = +1$
- d. $FC(N) = +1$ and $FC(B) = 0$
- e. $FC(N) = 0$ and $FC(B) = +1$

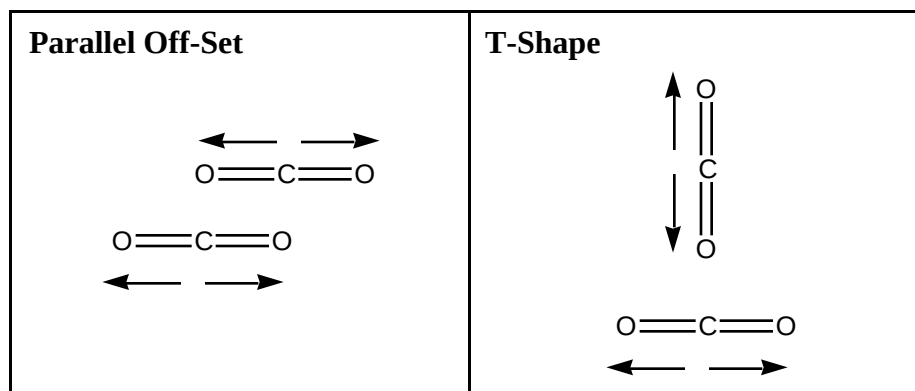
Question 3. Intermolecular Interactions. (12 points)

The article “TANKER BLEEDS OIL IN TOKYO BAY. WORST SPILL IN JAPAN'S HISTORY” (*AP and Reuters*, July 3, 1997) talked about oil spills and oil spill remediation and brings up the topic of **intermolecular bonding**. Oil and water don't mix because water does not want to. Alkanes interact with each other by way of van der Waals interactions only; these very weak forces are due to _____ (temporary, induced, permanent) dipoles in some alkanes inducing dipole moments in other alkanes. Alkanes would _____ (love, hate) to mix with water since such a mixture would replace the _____ (weak, strong) interactions between alkane molecules with _____ (weaker, **stronger**) dipole - _____ (temporary, **induced**, permanent) dipole interactions between water and alkane molecules, respectively. Water does not want to mix with alkanes because water would lose some strong hydrogen bonding interactions and this loss would not be compensated for by the water-alkane interactions.

Let's look at some examples of hydrogen-bonding that were presented in the visualization center accompanying “intermolecular bonding.” (I) Draw the structure of water dimer and indicate partial charges. (II) Draw the structure of ammonia dimer. (III) Draw a cyclic water trimer. For all cases I – III, always show all lone pairs and indicate H-bonds as dashed lines.



Let's look at the dimer of carbondioxide. Draw the “parallel off-set” and the “T-shape” structures. Indicate the bond dipole moments in the $O=C=O$ molecule.

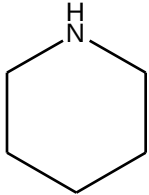
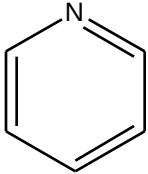
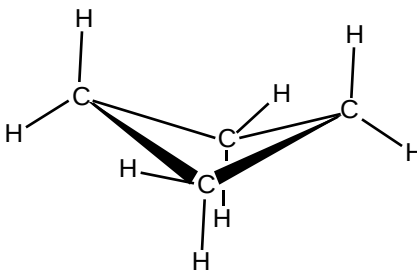
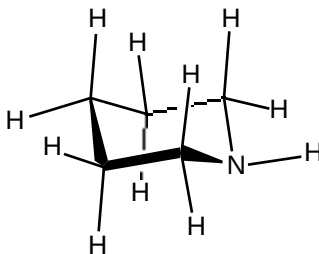
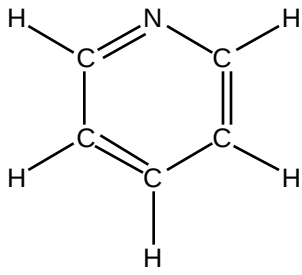


Question 4. Molecular Orbitals and Hybridization.. (16 points)

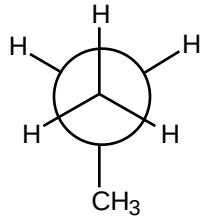
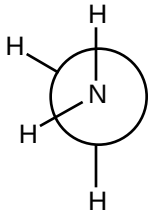
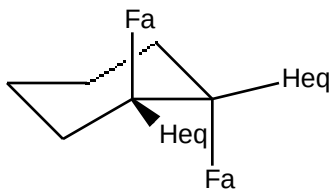
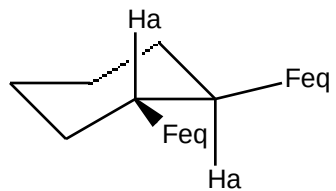
- E-Q6 How many node planes are there in the antibonding sigma MO that is constructed by overlap between two p-AOs?
- a. 0 node planes
 - b. 1 node plane created by the anti-bonding combination
 - c. 2 node planes, the ones that are always present in p-AOs
 - d. 3 node planes, all the planes mentioned in (b) and (c)**
 - e. 2 node planes and 1 airplane
- E-Q9 Based on what you know about sp^n hybrid orbitals, can you abstract and define the meaning of an spd-hybrid orbital?
- a. contains one s-, one p-, and one d-atomic orbital
 - b. contains one half s-AO, one half p-AO, and one half d-AO
 - c. contains one quarter s-AO, one third p-AO, and one fifth d-AO
 - d. contains a third of s-, p-, and d-AOs**
 - e. contains a quarter of s-, p-, and d-AOs
- E-Q12 If the sigma bonds of formaldehyde, H_2CO , are in the xy-plane, which of the three p-AOs are employed to construct the π -bond?
- a. p_x -AOs alone
 - b. p_z -AOs alone**
 - c. p_x -AOs and p_z -AOs in equal parts
 - d. p_y -AOs alone
 - e. p_y -AOs and p_z -AOs in equal parts
- E-Q13 For the N-atom in HCN, what is the best single representation of its electron configuration after promotion and hybridization? (Note that the N in HCN has one lone pair!)
- a. $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$
 - b. $1s^2 2sp_x^2 2sp_x^1 2p_y^1 2p_z^1$**
 - c. $1s^2 2(sp^2)^2 2(sp^2)^1 2(sp^2)^1 2p_z^1$
 - d. $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^0$
 - e. $1s^2 2sp_x^2 2sp_x^2 2p_y^1 2p_z^0$

Question 5. Structures and Representations of Molecules. (14 points)

Three bond-line diagrams are shown. In the boxes below each of the diagrams, provide a perspective drawing of the molecule that shows all atoms and that shows the correct 3-dimensional geometry.

Provide structural drawings as requested.

Newman projection of propane 	Newman projection of hydrazine 
<i>Trans</i> 1,2-difluorocyclohexane, less stable conformation, perspective drawing 	<i>Trans</i> 1,2-difluorocyclohexane, most stable conformation, perspective drawing 

Question 6. Alkanes. (16 points)

PE1-Q6 What is the technical name of the process by which long-chain alkanes are thermally broken down, in the presence of hydrogen gas, to shorter chain hydrocarbons?

- a. Reforming
- b. Cracking
- c. **Hydrocracking**
- d. Distillation
- e. Refining

PE1-Q7 Which reaction describes the complete combustion of cyclopropane?

- a. **$\text{C}_3\text{H}_6 + 4.5 \text{O}_2 \rightarrow 3 \text{CO}_2 + 3 \text{H}_2\text{O}$**
- b. $\text{C}_3\text{H}_6 + 3.0 \text{O}_2 \rightarrow 3 \text{CO} + 3 \text{H}_2\text{O}$
- c. $\text{C}_3\text{H}_6 + 4.5 \text{O}_2 \rightarrow 2 \text{CO}_2 + 3 \text{H}_2\text{CO} + 2 \text{H}_2\text{O}$
- d. $\text{C}_3\text{H}_8 + 5 \text{O}_2 \rightarrow 3 \text{CO}_2 + 4 \text{H}_2\text{O}$
- e. $\text{C}_3\text{H}_8 + 3.5 \text{O}_2 \rightarrow 3 \text{CO} + 4 \text{H}_2\text{O}$

PE1-Q9 Which statement best describes the C-C-C-C conformations in the boat and twist-boat conformations of cyclohexane?

- a. Two *cis* conformations and two *anti* conformations.
- b. Two *anti* conformations and two *gauche* conformations.
- c. Four *cis* conformations and two *gauche* conformations.
- d. **Two *cis* conformations and four *gauche* conformations.**
- e. Two *cis* conformations and four *anti* conformations.

PE1-Q13 Monosubstituted cyclohexanes exist as equilibria between axial and equatorial conformers. Select the molecule with the least concentration of axially substituted cyclohexane.

- a. ethylhexane
- b. propylcyclohexane
- c. isopropylcyclohexane
- d. *sec.*-butylcyclohexane
- e. ***tert.*-butylcyclohexane**

Question 7. Energy Profile for Ring Flipping in Cyclohexane. (12 points)

The energy profile is drawn schematically for the ring flipping in cyclohexane and with the center section omitted. Complete the energy profile. Indicate which point(s) on the diagram correspond to “half-chair,” “twist-boat” and “boat” conformations (write appropriate word into diagram). Provide good estimates for the highest activation energy and for the energy of the “twist boat” relative to the “chair.” Finally, draw Newman projections of the “chair” and “boat” conformations of cyclohexane.

