

Chemistry 210  
“Organic Chemistry I”  
Fall Semester 2000  
Dr. Rainer Glaser

Examination #1

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

Friday, September 22, 2000, 9:00 - 9:50

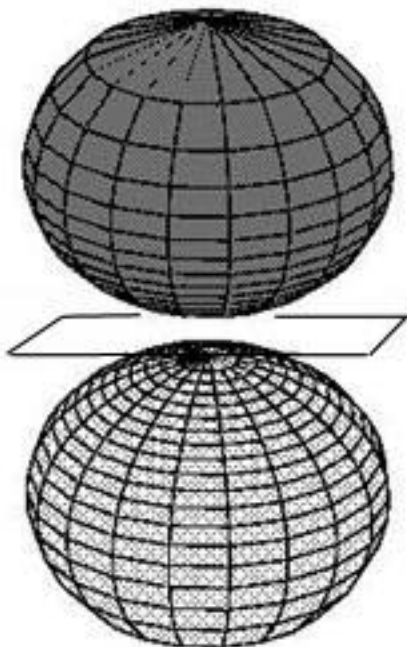
Name:

*Answer Key*

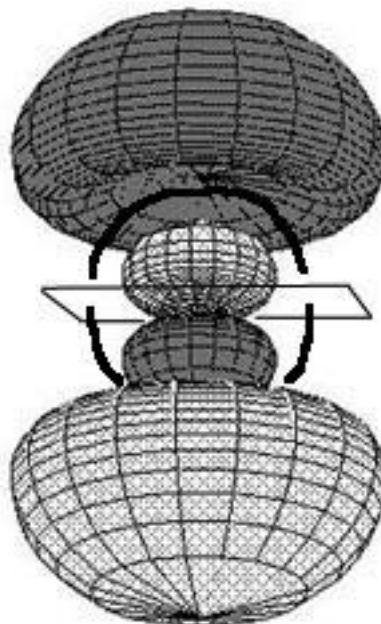
Question 1. Carbon and Atomic Orbitals.	20	
Question 2. LK Structures & Hybridization (News #1).	20	
Question 3. Intermolecular Interactions (News #2).	20	
Question 4. Alkanes and Combustion.	20	
Question 5. Conformations of Ethane and Butane.	20	
Total	100	

**Question 1.** Carbon and Atomic Orbitals. (20 points)

Assume that the “z-axis” coincides with the vertical direction.



This above picture shows the  $2p_z$  AO.  
The main quantum number is  $n = 2$ .  
The second quantum number is  $l = 1$ .  
There are 1 node planes (draw them, if any).  
There are 0 node spheres (draw them, if any).  
(5 points)



This above picture shows the  $3p_z$  AO.  
The main quantum number is  $n = 3$ .  
The second quantum number is  $l = 1$ .  
There are 1 node planes (draw them, if any).  
There are 1 node spheres (draw them, if any).  
(5 points)

What is the ground state electron configuration of carbon? (5 points)

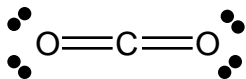
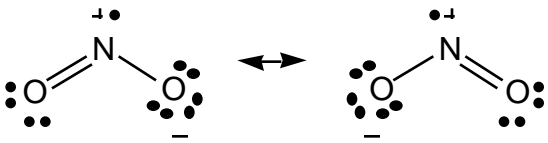
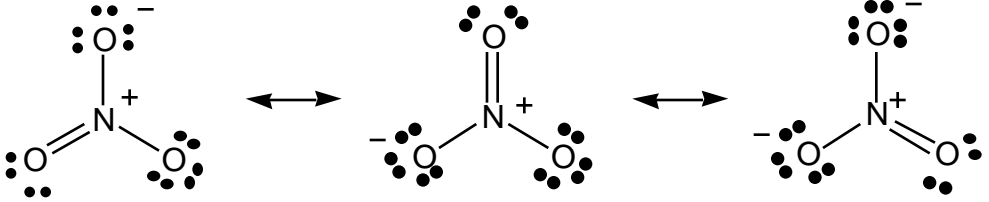
- (a)  $1s^2 2s^2 2p^0$  (b)  $1s^2 2s^2 2p^1$  (c)  **$1s^2 2s^2 2p^2$**  (d)  $1s^2 2s^2 2p^3$  (e)  $1s^2 2s^2 2p^4$

Which isotope of carbon is used in “carbon dating”? (5 points)

- (a)  $^{10}\text{C}$  (b)  $^{11}\text{C}$  (c)  $^{12}\text{C}$  (d)  $^{13}\text{C}$  (e)  **$^{14}\text{C}$**

**Question 2.** Lewis-Kekule Structures & Hybridization. (20 points)

The article “U.S. FLOATS NEW 'BUBBLE' PROPOSAL” (*Asahi News Service*, December 11, 1997) brought up some timely issues in atmospheric chemistry. Carbon dioxide, nitrogenoxide, nitrogen dioxide, and nitric acid were among the molecules responsible for the greenhouse effect. For each of these molecules shown, provide the Lewis-Kekule structure. If several resonance forms are needed for the proper description of the molecule, then you should provide all the major resonance forms. In all cases, clearly indicate formal charges (if any).

<p><b>CO<sub>2</sub></b> (4 p)</p>  <p>Total number of valence electrons: <u>16</u></p> <p>Radical? Yes - <b>No</b> (Circle one)</p>	<p><b>NO<sub>2</sub></b> (4 p) (RFs with rad. at O also are possible)</p>  <p>Total number of valence electrons: <u>17</u></p> <p>Radical? <b>Yes</b> - No (Circle one)</p>
<p><b>NO<sub>3</sub><sup>-</sup></b> (4 p)</p> 	

The hybridization of the C-atom in carbon dioxide (2 p):

**sp**

The hybridization of the N atom in NO<sub>2</sub> (2 p):

**sp<sup>2</sup>**

The O-C-O angle in carbon dioxide (2 p):

**180°**

The approximate O-N-O angle in nitrogen dioxide (2 p):

**about 120°**

**Question 3.** Intermolecular Interactions. (20 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 modern ways of oil spill remediation. Oil spill remediation is based on the optimal use of knowledge about **intermolecular bonding**.

What is the dominant interaction between octane molecules in condensed phase? (5 points)

- (a) charge-charge interaction
- (b) charge-dipole interaction
- (c) dipole-dipole interaction
- (d) hydrogen bonding
- (e) van der Waals interactions**

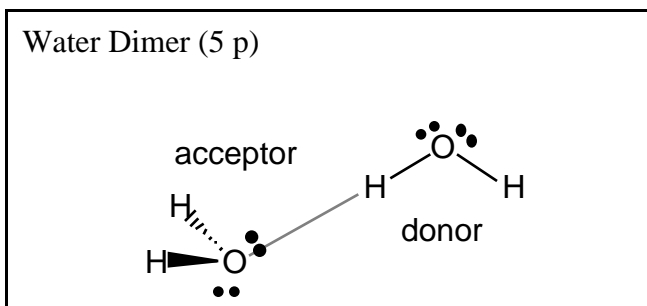
What is the value of the electronegativity of oxygen atom? (2.5 points)

- (a) 4.0
- (b) 3.5**
- (c) 3.0
- (d) 2.5
- (e) 2.0

What is the approximate value of the electronegativity of hydrogen atom? (2.5 points)

- (a) 4.0
- (b) 3.5
- (c) 3.0
- (d) 2.5
- (e) 2.0**

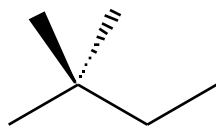
Draw a hydrogen-bonded dimer of water as accurately as you can. Show all lone pairs. Indicate the hydrogen bond by dashes. Indicate who is the hydrogen bond donor and who is the hydrogen bond acceptor. Indicate the polarity of the OH bonds using partial charges  $+$  and  $-$ . (5 p)



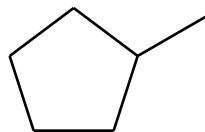
Why does octane not mix with water? (5 points, be brief and concise)

Water likes to bind with water very much, water has no benefit from binding octane.  
Octane binds weakly to octane. Octane binds more strongly to water, would love to bind to water!  
Octane wants to dissolve in water, water does not want to mix with octane.

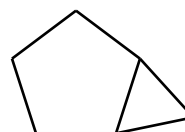
**Question 4.** Alkanes and Combustion. (20 points)



**1**



**2**



**3**

Provide a name for **1** (3 p): 2,2-dimethylbutane

Provide a name for **2** (3 p): methylcyclopentane

Provide a name for **3** (3 p): bicyclo[3.1.0]hexane

Provide the molecular formula for **1** (1 p):  $C_6H_{14}$

Provide the molecular formula for **2** (1 p):  $C_6H_{12}$

Provide the molecular formula for **3** (1 p):  $C_6H_{10}$

Provide the empirical formula for **3** (1 p):  $C_3H_5$

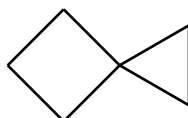
Draw a small circle around every tertiary carbon atom in molecules **1 – 3**. (1 p)

Draw a small square around every  $4^\circ$  carbon in molecules **1 – 3**. (1 p)

Provide a stoichiometric equation for the combustion of compound **3** (2 p):



Draw the structure of spiro[3.2]hexane (3 p):

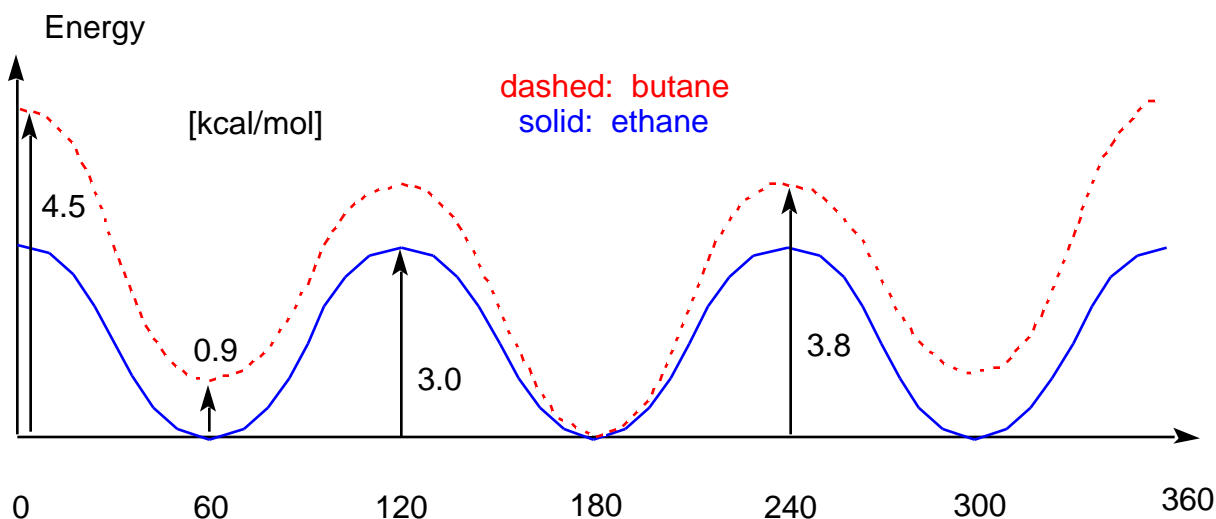


**Question 5.** Rotational Energy Profiles of Ethane and Butane. (20 points)

(a) Draw the rotational energy diagram for **ethane**,  $\text{H}_3\text{C}-\text{CH}_3$ . Begin the diagram on the left with the eclipsed structure of ethane and draw the rotational energy profile. Provide the energy difference between the staggered and the eclipsed conformations: 3 kcal/mol. (5 points)

(b) Next, draw the rotational energy diagram for **butane**,  $\text{H}_3\text{C}-\text{H}_2\text{C}-\text{CH}_2-\text{CH}_3$  about the central CC bond. Begin the diagram on the left with the eclipsed structure that has the two methyl groups in a *cis* arrangement (dihedral angle 0). Draw the rotational energy profile of butane as accurately as possible, that is, I would like to see the correct ordering between the various minima and the various transition state structures. But there is no need to provide the actual energy differences. (5 points)

(c) Draw the requested Newman projections in the boxes below. (10 points)



**Draw the Newman Projections in these spaces.**

Staggered ethane (2 p)	Eclipsed ethane (2 p)	<u>Most stable structure of staggered butane</u> (3 p)	<u>Least stable structure of eclipsed butane</u> (3 p)
