Chem 2100, "Organic Chemistry I"
WS07, Dr. Rainer Glaser

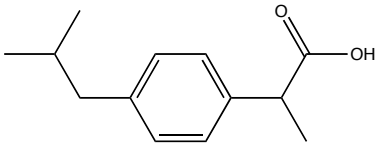
Exam #1
"AO, HAOs, MOs, Intra- & Intermolecular Bonding. Sources, Properties, and Uses of Acyclic Alkanes."

Friday, 2-23-2007, 9:00-9:55 am

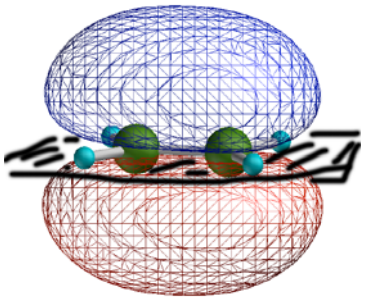
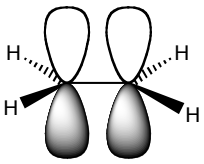
Name: Answer Key

Question 1. Geometry, Hybridization & MOs.	20	
Question 2. Intermolecular Interactions.	20	
Question 3. Nomenclature of Alkanes.	20	
Question 4. Alkanes and Energy Production.	20	
Question 5. Conformations of Alkanes.	20	
Total	100	

Question 1. Geometry, Hybridization & MOs. (20 points)

(a) Ibuprofen, reduces inflammation and fever by blocking prostaglandin cyclooxygenase, an enzyme that catalyzes the formation of prostaglandins, hormone-like chemicals involved in tissue inflammation and repair. (6 p.)	
Approximate length of the C=O double bond (with units)?	**1.2 Å** or **120 pm**
Hybridization of the C-atom that carries the *iso*-butyl group?	**sp^2**
Number of sp^2-hybridized C-atoms?	**7** (6 in ring & COOH)
Number of lone pairs on the O-atom of the OH group?	**2**
Hybridization of the O-atom of the C=O group.	**sp^2**
Number of primary (1˚) C-atoms?	**3**

(b) Ethene has σ- and π-bonds. The π-MO shown is formed by LCAO of the carbon p-AOs that are perpendicular to the plane of the molecule and the colors indicate different orbital signs. (6 points)

	Draw a "lobe diagram" of the π-MO (i.e. use ): 	Number of node planes: _**1**_. If there are any, then draw them in the picture on the left and in your lobe diagram. How many electrons occupy this MO in the ground state? _**2**_

(c) Acetylene, C_2H_2. (8 points)

Provide the complete Lewis-Kekule structure and provide the value(s) of the HCC angles: H–C≡C–H, ∠(H-C-C) = 180°	What kinds of carbon orbitals are used to form the molecular orbital for the CC σ-bond? C(sp) and C(sp)
Which carbon and hydrogen orbitals are used to construct the CH σ-bond? C(sp) and H(s)	What kinds of carbon orbitals are used to form the molecular orbital for one of the CC π-bonds? C(p_x) and C(p_x)

Question 2. Intermolecular Interactions. (20 points)

(a) What is the primary interaction responsible for **hydrogen-bonding**? (2 points)

(a) temporary dipole / induced dipole (TI)

(b) induced dipole / induced dipole (II)

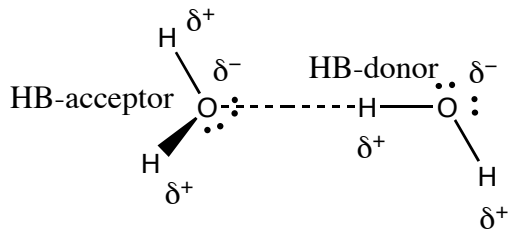
(c) temporary dipole / permanent dipole (TP)

(d) induced dipole / permanent dipole (IP)

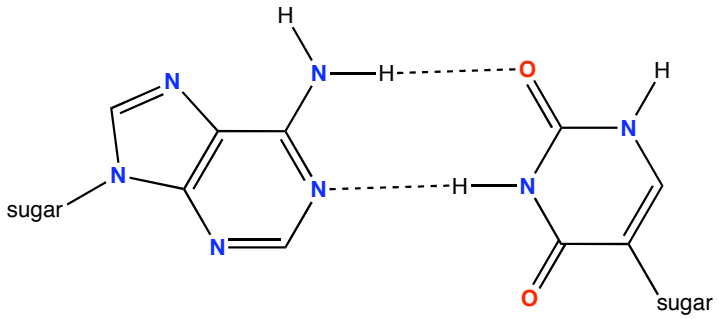
(e) permanent dipole / permanent dipole (PP)

(b) Draw a hydrogen-bonded dimer of water. Show all lone pairs. Indicate the hydrogen bonds by dotted lines. Indicate who is the hydrogen bond donor and who is the hydrogen bond acceptor. Indicate the polarity of the OH bonds using partial charges δ^+ and δ^-. Show relative distances and angles as accurate as possible. (8 points)

Water Dimer



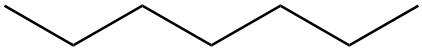
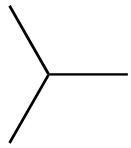
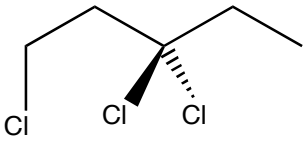
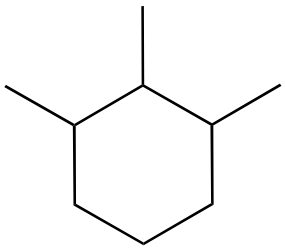
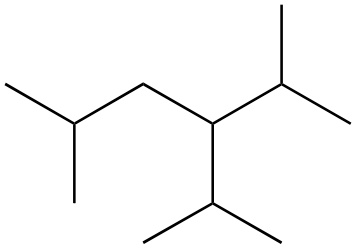
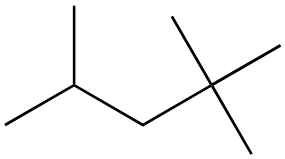
(c) Complete the Lewis-Kekule structure of the adenine-thymine base pair by adding all lone pairs. Then, using dotted lines, indicate the hydrogen bond(s) that bind(s) these two DNA bases. (4 points)



(d) Octane _____ (does, ***does not***) mix with water. Octane would _____ (***love***, hate, be indifferent) to mix with water because its ____ (PP, ***IP***, TP, II, IT) interactions with water are _____ (***stronger***, weaker, about the same) than/as ____ (PP, IP, TP, II, ***IT***) interactions between octane molecules. Yet, water interacts _____ (***better***, about the same, worse) with other water molecules and therefore water molecules would _____ (love, ***hate***, be indifferent) to mix with octane molecules. (6 points)

Question 3. Nomenclature of Alkanes. (20 points)

Where the structure is given, provide an acceptable name. Where the names is given, provide an acceptable structure (complete, condensed, line drawing… are fine as long as the structure is correct).

 *n*-heptane	Isobutane 
 1,3,3,-trichloropentane	1,2,3-trimethylcyclohexane 
 3-isopropyl-2,5-dimethylhexane	2,2,4-trimethylpentane 

Question 4. Alkanes and Energy Production. (20 points)

(a) Provide a stoichiometric equation for the ***complete*** combustion of butane. (4 points)

$$C_4H_{10} + 6.5\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$$

(b) Suppose you combust 1 kg of butane. How many kg of CO_2 are formed? How many liters of CO_2 are formed. (6 points)

Molmass(C_4H_{10}) = 4 x 12 + 10 = 58 g/mol. 1 kg butane contains 17.24 moles.
Each mole of butane yields 4 moles of CO_2. Total CO_2 produced: 69 moles with volume 22.4 l/mol.
Molmass(CO_2) = 12 + 2 x 16 = 44 g/mol. Total CO_2 produced: 3,036 kg or 1546 liters.

(c) Provide a stoichiometric equation for the ***incomplete*** combustion of methane (i.e. natural gas) to carbon monoxide. (4 p.)

$$CH_4 + 1.5\ O_2 \rightarrow CO + 2\ H_2O$$

(d) In a few sentences and using chemical reaction equations as needed, compare and contrast the use of hydrogen gas in "combustion engines" and in "fuel cells." (6 points)

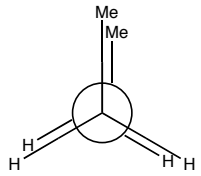
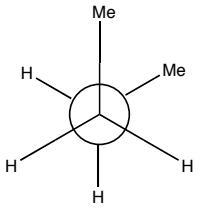
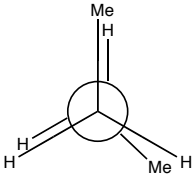
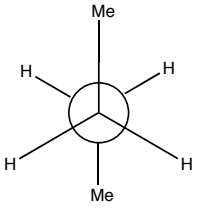
Combustion Engine: $2\ H_2 + O_2$ -(mix, burn with flame)→ $2\ H_2O$ + kinetic energy / heat

Fuel Cell: $2\ H_2 + O_2$ -(no flame)→ $2\ H_2O$ + electrical energy

Fuel cells are more efficient because the chemical energy is converted directly into electrical power and there is very little energy lost to unwanted heating.

Question 5. Conformations of Alkanes. (20 points)

(a) Draw the **Newman projections for butane** with C-C-C-C dihedral angles 0°, 60°, 120°, and 180°. Indicate which ones are "eclipsed" and which ones are "staggered." Indicate the name of the conformation (*i.e.* "cis" etc.) inside the respective box. (12 points)

dihedral angle = 0°  eclipsed, cis	dihedral angle = 60°  staggered, gauche
dihedral angle = 120°  eclipsed, no special name	dihedral angle = 180°  staggered, trans

(b) Draw a schematic energy diagram is shown for the rotational profile of butane. Provide the energy values in kcal/mol and indicate which points correspond to which conformations. (8 points)