EXAM 1

CHEMISTRY 220a

Friday, September 24, 2004

NAME (print): _____

TA:_____ Day:_____ Time:_____

Take a few moments to look over the exam. Answer each question on the exam paper.

Important clues and structures are in **bold**.

Do all **preliminary** drawing or computations on the work sheets at the end of the exam. The work sheets will not be graded.

The exam is 55 minutes.

STOP writing and hand in your exam when you are asked to do so.

REMEMBER: Neatness is to your advantage.

1. Structure/Conformation (30 pts) _____

2. Conformation (20 pts) _____

3. Potpourri (30 pts) _____

4. Orbitals (20 pts) _____

_____

Total (100 pts)

1. **Structure/Conformation** (30 pts): Limonene, which is isolated from lemon grass, is a **C_{10} hydrocarbon** that contains a 6-membered ring and two double bonds.

   a) (5 pts) In addition to carbon, what other atoms are present in limonene and how many are there of each kind? Show your reasoning.

Addition of hydrogen to the double bonds of limonene (alkene → alkane) produces two 1,4-disubstituted cyclohexane stereoisomers, **A** ($C_{10}H_{20}$) and **B**.

b) (5 pts) What is the formula of **B**? Why?

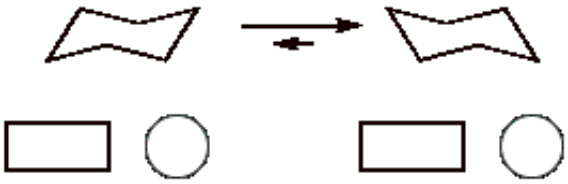
Continued …

Compound **A** has an energy difference of 3.8 kcal/mol between its two chair conformations $\mathbf{A_{major}}$ and $\mathbf{A_{minor}}$. Compound **B** has an energy difference of 0.4 kcal/mol between its chair

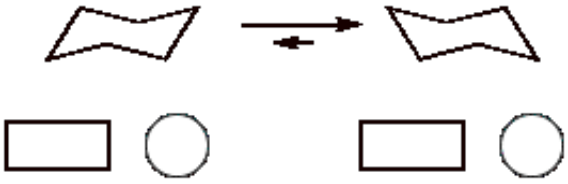
conformations $\mathbf{B_{major}}$ and $\mathbf{B_{minor}}$.

c) (20 pts) Using the relevant data below, determine the structures of $\mathbf{A_{major}}$, $\mathbf{A_{minor}}$, $\mathbf{B_{major}}$, and $\mathbf{B_{minor}}$. Place the substituents on the chair templates in their correct positions and configurations (pay attention to the equilibria), enter the energy in each box, and the designations ($\mathbf{A_{major}}$, $\mathbf{A_{minor}}$, $\mathbf{B_{major}}$, and $\mathbf{B_{minor}}$) in the circles. Values [DGo (kcal/mol)] for energy differences between axial and equatorial isomers of mono-substituted cyclohexanes are as follows: -CN, 0.2; -COOH, 1.4; -CH3, 1.7; -CH2CH3, 1.8; $-CH(CH_3)_2$, 2.1; $-C(CH_3)_3$, 5.4.] **Show work.**

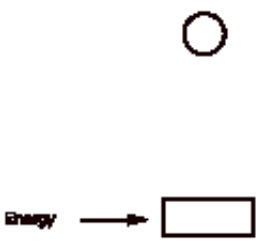
Compound **A**:

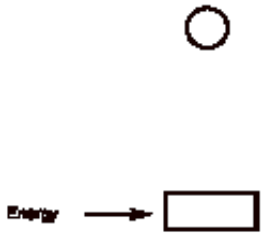


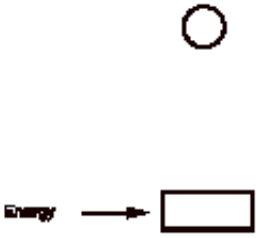
Compound **B**:



2. **Conformation** (20 pts): Draw Newman projections of the three most stable conformations of 2,3-dimethylpentane viewed along the C2-C3 sigma bond. Use the **circles** as templates for the Newman projections. Calculate the energy (kcal/mol) of each conformation. Place your answer in the appropriate **box**. **Show work.** [H/H, eclipsed, 1.0 kcal/mol; CH3/H eclipsed, 1.3 kcal/mol; C2H5/H, eclipsed, 1.4 kcal/mol; CH3/CH3, eclipsed, 3.0 kcal/mol; CH3/CH3, gauche, 0.9 kcal/mol; CH3/C2H5, gauche, 1.0 kcal/mol.]







3. **Potpourri** (6 x 5 pts = 30 pts.; equal weight):

a) **Circle** the C_1-C_4 dihedral (torsional) angle in the highest energy conformation of n-butane.

0° 60°` 120° 180° 270°

b) **Circle** the compound C_8H_{18} having the **most negative** heat of formation and the **smallest difference** between its mp and bp (5.6 °C).

n-octane 2,2,3,3-tetramethylbutane 2,2-dimethylhexane

2,3-dimethylhexane 2,3,4-trimethylpentane

c) **Circle** the acid that is ranked third in relative pKa.

CH_4 CH_3OH NH_3 NH_4^+ CH_3CO_2H

d) **Circle** the compounds that contain atoms with sp hybridization.

acetylene ethyne CO_2 HCN BeH_2

e) **Circle** the compounds with net dipole moments.

$BrCH_2CH_2Br$ cyclohexane BrHC=C=CHBr propane $HCBr_3$

f) **Circle** the species in which resonance plays a role.

RCO_2^- CH_3ONa $CH_2=CHCH_2^+$ $CH_3CH_2CH_2^+$ $^+CH_2CH_2N(CH_3)_2$

4. **Orbitals** (20 pts): Provide a molecular orbital representation of acrylonitrile (CH_2=CHCN). Include pi-bonds, p-orbitals, and non-bonding electrons. Identify the hybridization of each carbon. You may use lines for sigma bonds. Provide necessary commentary.

Work Sheets
Work Sheets
Work Sheets