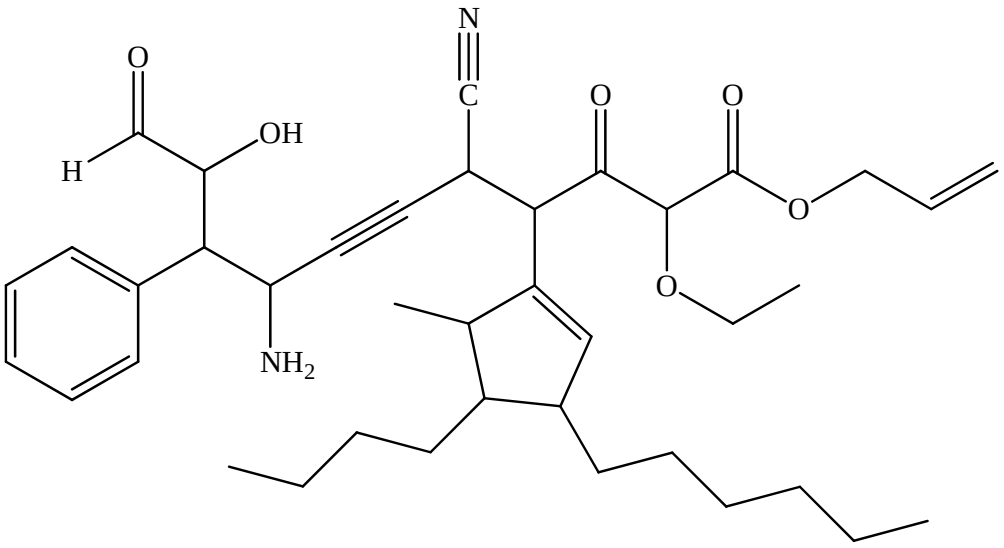
Chem 201 Midterm
Winter, 2013 Name _____
Beauchamp

Problems	Points	Credit
1. Functional Group Nomenclature	25	
2. Degrees of Unsaturation & Functional Groups or Various Nomenclature Terms	15	
3. 2D structure, Functional Groups	20	
4. 2D / 3D Resonance Structures, Formal Charge	25	
5. Simple 2D Resonance Structures, Formal Charge	12	
6. Physical Properties, Forces of Interaction	15	
7. Cyclohexane Conformations, Substituents, Energy, K_{eq}.	25	
8. Newman Projections, Open Chain Structure, Relative Energies, K_{eq}.	20	
9. Stereochemical Analysis	25	
Total	182	

This is a long exam. It has been designed so that no one question will make or break you. The best strategy is to work steadily, starting with those problems you understand best. Make sure you show all of your work. Draw in any lone pairs of electrons, formal charge and curved arrows to show electron movement where appropriate. I give partial credit, so writing down anything that you know is correct will be helping yourself. Do your best to show me what you know in the time available.

In the middle of every difficulty lies opportunity. Albert Einstein

1. Provide an acceptable name for the following molecule. (25 pts)



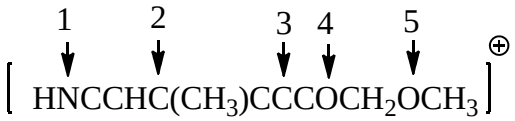
2. Use the given molecular formula to calculate the degree of unsaturation. Draw an example molecule that has the indicated functional groups. (15 pts)

   $C_{25}H_{27}BrClNO_7S_2$, functional groups: carboxylic acid, anhydride, thiol, sulfide, amide, alkyne, ring, bromo, aromatic, acid chloride

3. Draw an acceptable Lewis structure (2D) for the following formula. Show <u>all</u> single, double and triple bonds with one, two or three lines. Include all lone pairs of electrons as two dots. Include formal charge, if present at the atom where present. Identify any functional groups by name (i.e. ketone, amide, etc.) (20 pts)

$$\left[(CH_3)_2NOCCHCHCCCOCH_2CO_2CH(CO_2H)CHOHC_6H_4CHNH_3CH(OCH_3)CHO \right]^{\oplus}$$

4. First draw a 2D Lewis structure and one additional resonance structure of the following molecule (there are 4 total, include the best). Draw one correct 3D structure. Show bonds in front of the page as wedges, bonds in back of the page as dashed lines and bonds in the page as simple lines. Show orbital representations for pi bonds and lone pairs along with their electrons. Fill in the informational table at the bottom for the numbered atoms. (25 pts)



2D

3D

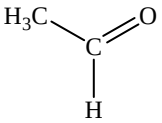
Atom	Shape	Hybridization	Bond Angles	#σ bonds	#π bonds	# lone pairs
1						
2						
3						
4						
5						

5. Draw all 2D resonance structures for the following structures. Assume full octets for all nonhydrogen atoms unless there is a positive charge written. Use correct arrows, formal charge and include lone pairs. (6 pts each)

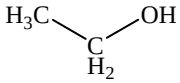
a. $HCCCH_2^{\oplus}$

b. CH_2CHO

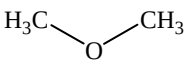
6. Match the given boiling points with the structures below and give a short reason for your answers. (-42°C, -22°C, +20 °C, +78 °C, +101°C, 1380°C) (15 pts)



ethanal
MW = 44 g/mol



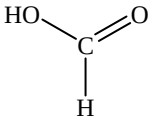
ethanol
MW = 46 g/mol



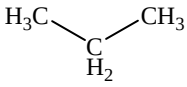
dimethylether
MW = 46 g/mol

Li Cl

lithium chloride
MW = 42.4 g/mol



ethanoic acid
MW = 46 g/mol



propane
MW = 44 g/mol

7. Draw all possible chair conformations of trans-1-phenyl-2-chlorocyclohexane. Which conformation is more stable? Draw it first. Provide a reason for your answer. Draw Newman projections of both conformations using the $C_1 \rightarrow C_2$ and $C_5 \rightarrow C_4$ bonds to sight along. Point out any gauche interactions shown in your Newman projections. Assume any gauche interaction of side chain groups is 0.8 kcal/mole, combined with any axial energy values (see table) to determine the relative percents of each conformation. Sketch an energy diagram that shows how the energy changes with the conformational changes. Assume a single boat transition state, TS (you do not have to draw the boat) (25 pts)

Given Information

Substituent	ΔG^o (A value)	Substituent	ΔG^o (A value)
-H	0.0	-F	0.3
$-CH_3$	1.7	-Cl	0.5
$-CH_2CH_3$	1.8	-Br	0.5
$-CH(CH_3)_2$	2.1	-I	0.5
$-C(CH_3)_3$	> 5.0	$-C_6H_5$ (phenyl)	2.9

chair 1 $\rightleftharpoons$ chair 2

$$K = \frac{\text{chair 2}}{\text{chair 1}} = 10^{\frac{-\Delta G}{2.3RT}}$$

R = 2 cal/(mole-K)
T ≈ 300 K

chair 1
(most stable)

trans-1-phenyl-2-chlorocyclohexane

chair 2
(less stable)

Newman projections:

$C_1 \rightarrow C_2$ and $C_5 \rightarrow C_4$

$C_1 \rightarrow C_2$ and $C_5 \rightarrow C_4$

$C_1 \rightarrow C_2$ and $C_5 \rightarrow C_4$

$$K = \frac{\text{chair 2}}{\text{chair 1}} = 10^{\frac{-\Delta G}{2.3RT}} =$$

Energy changes of trans-1-phenyl-2-chlorocyclohexane conformations.

8. Use a Newman projection of the C3→C4 bond of 3-methyl-4-phenylhexane to **show the most stable conformation first**. Rotate through all of the eclipsed and staggered conformations. Using the energy values provided in the table below, calculate the relative energies of the different conformations. Plot the changes in energy in the graph diagram provided. Hint: Draw a 2D structure first and "bold" the bond viewed in your Newman projection, then decide your line of sight. (This is the way your question will read on the final exam. On the midterm exam you will only have to draw the highest energy conformation and the lowest energy conformation.) (20 pts)

2D structure

$\Delta G \approx \Delta H$

$K_{eq} = 10^{\frac{-\Delta H}{2.3RT}}$

Approximate Eclipsing Energy Values (kcal/mole)

	H	Me	Et	i-Pr	t-Bu	Ph
H	1.0	1.4	1.5	1.6	3.0	1.7
Me	1.4	2.5	2.7	3.0	8.5	3.3
Et	1.5	2.7	3.3	4.5	10.0	3.8
i-Pr	1.6	3.0	4.5	7.8	13.0	8.1
t-Bu	3.0	8.5	10.0	13.0	23.0	13.5
Ph	1.7	3.3	3.8	8.1	13.5	8.3

Approximate Gauche Energy Values (kcal/mole)

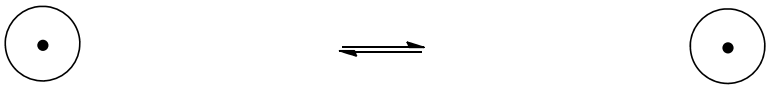
	H	Me	Et	i-Pr	t-Bu	Ph
H	0	0	0.1	0.2	0.5	0.2
Me	0	0.8	0.9	1.1	2.7	1.4
Et	0.1	0.9	1.1	1.6	3.0	1.5
i-Pr	0.2	1.1	1.6	2.0	4.1	2.1
t-Bu	0.5	2.7	3.0	4.1	8.2	3.9
Ph	0.2	1.4	1.5	2.1	3.9	2.3

most stable conformation

least stable conformation

$\Delta H^o =$

$\Delta H^o =$



$K_{eq} = 10^{\frac{-\Delta H}{2.3RT}} =$

9. Use the given formula to illustrate the requested example. Formula = $C_6H_{10}Br_2$ (25 pts)

a. Draw a 3D structure with one chiral center and its enantiomer. Specify chiral centers as R or S.

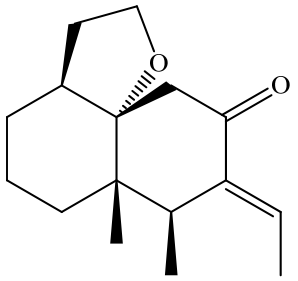
b. Draw a 3D structure with two chiral centers and its enantiomer. Specify chiral centers as R or S.

c. Draw a 3D structure with two chiral centers and a diastereomer. Specify chiral centers as R or S.

d. Draw two structures that do not have any chiral centers, but are stereoisomers.

e. Draw a structure that has chiral centers, but is not chiral.

f. Circle all stereogenic centers in following molecule and calculate the maximum number of stereoisomers possible.



You cannot teach people anything. You can only help them discover it within themselves. Galileo