Exam #1

Chemistry 333

Principles of Organic Chemistry I

Tuesday March 14, 2006

Name:_____.

The exam is worth a total of 100 points; there are five questions. Please show all work to receive full credit for an answer.

By putting your name on this exam, you agree to abide by California State University, Northridge policies of academic honesty and integrity
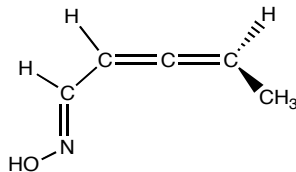
Molecular models are allowed for this exam. Calculators are not needed.

Good Luck!

1. Use the IUPAC rules to write the systematic name for the following hydrocarbon. **Identify on your structure primary (1°), secondary, (2°), tertiary (3°), and quaternary (4°) carbon atoms**. (5 minutes, 10 pts)
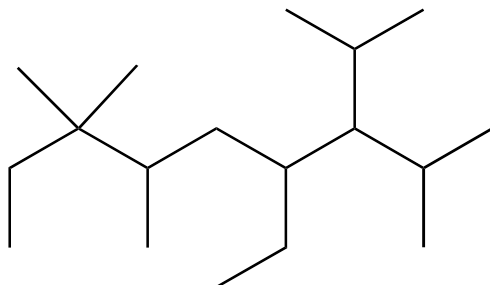
2. (20 pts, 15 minutes) For the following molecule:

a. Draw in all lone pairs and indicate the hybridization on all carbon, oxygen and nitrogen atoms present in the structure above. (5 points)

b. Draw a three-dimensional orbital diagram of this molecule, specifying all the orbitals on each atom that overlap to form bonds. *Remember to include lone pairs and indicate which orbitals they occupy.* Label the bonds as follows: σH_{1s}-C_{sp3} etc. Draw the sigma framework first, then the pi framework separately. (15 points)

3. Identify the relationship in the following pairs. Possibilites include: same molecules, constitutional isomers (structural isomers), diastereomers, enantiomers. (20 points) (10 minutes)

Relationship

a.

and

b.

and

c.

and

d.

and

e.

and
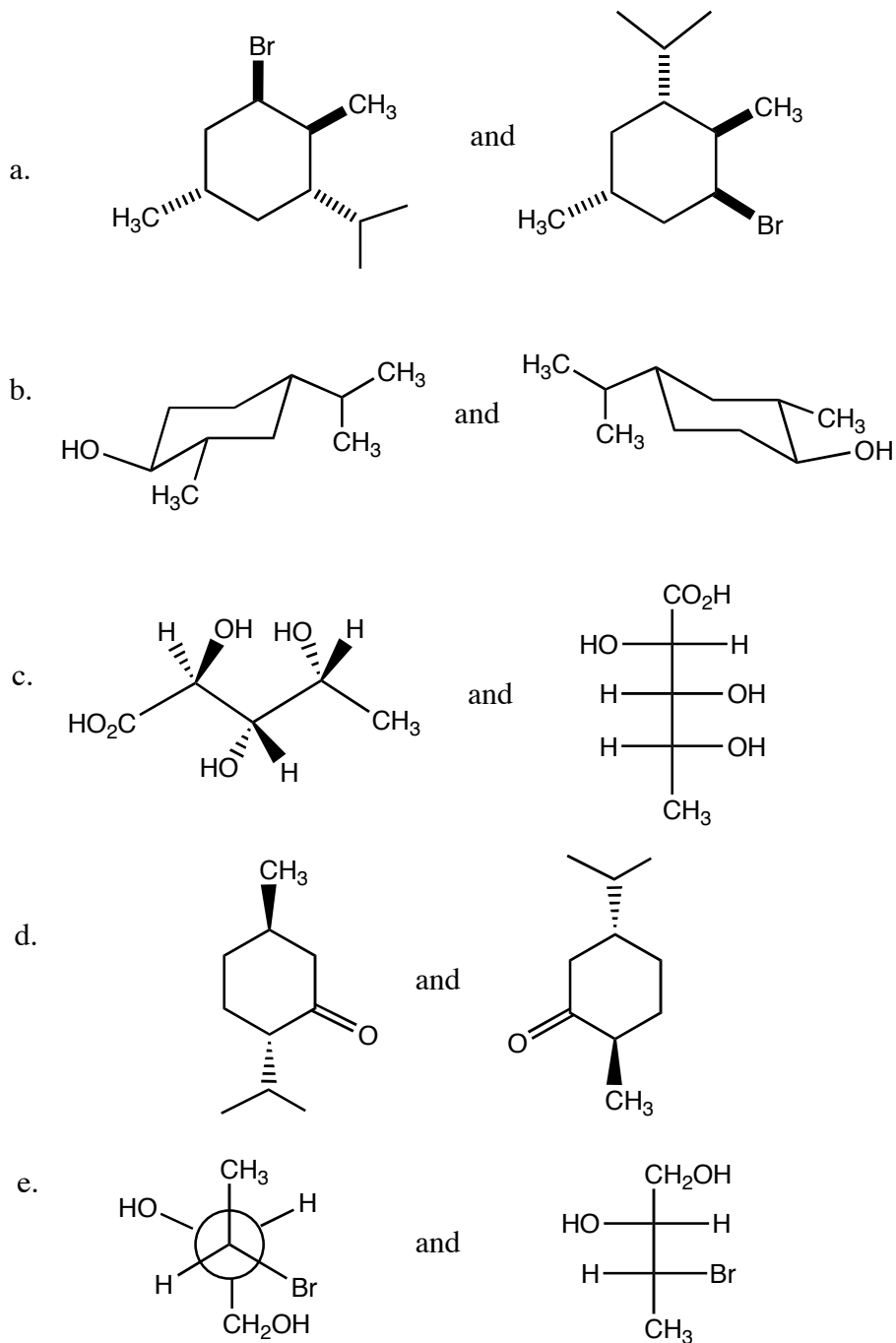
4. Use Fischer projections to draw <u>all</u> possible stereoisomers of 2-bromo-3-iodo butane. (20 points)
    a. Label pairs of compounds that are enantiomers or diastereomers
   b. assign configurations (**R** or **S**) for all asymmetric carbon atoms in each structure you draw. (10 minutes)

c. If (2R, 3S)-2-bromo-3-iodobutane has $[\alpha]_D$= -22°, what will be the observed rotation for a solution containing 1 gram of (2R, 3S)-2-bromo-3-iodobutane and 3 grams of (2S, 3R)-2-bromo-3-iodobutane? (5 points)

5. Heating halides **1** or **2** in methanol produces allylic cation salt **A**, depicted as a resonance hydrid:
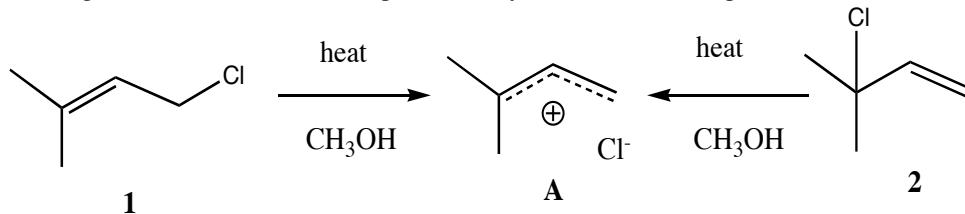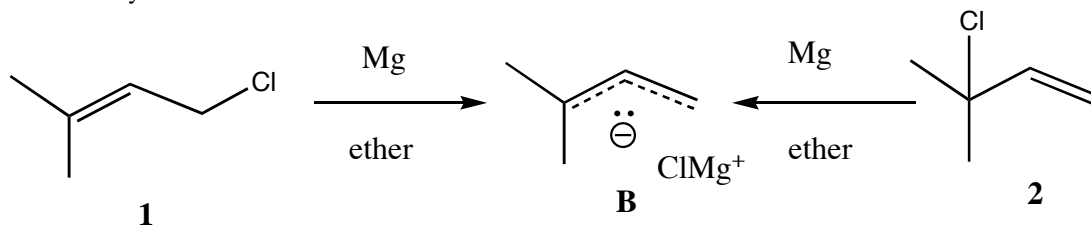

a.   Draw the individual resonance forms that contribute to resonance hybrid **A**, and indicate which is the major and which is (are) the minor resonance forms. Give a rationale for your assignment, discussing the relative **stabilities** of the resonance forms you have drawn.(5 points)

b. Based on your answer to (a), indicate which process occurs faster (i.e., has a more stable, lower energy **transition state**): **1➜ A** or **2➜ A**. Show this on the graph below, drawing transition state structures depicting the process of C-Cl bond cleavage in each case. (10 pts)
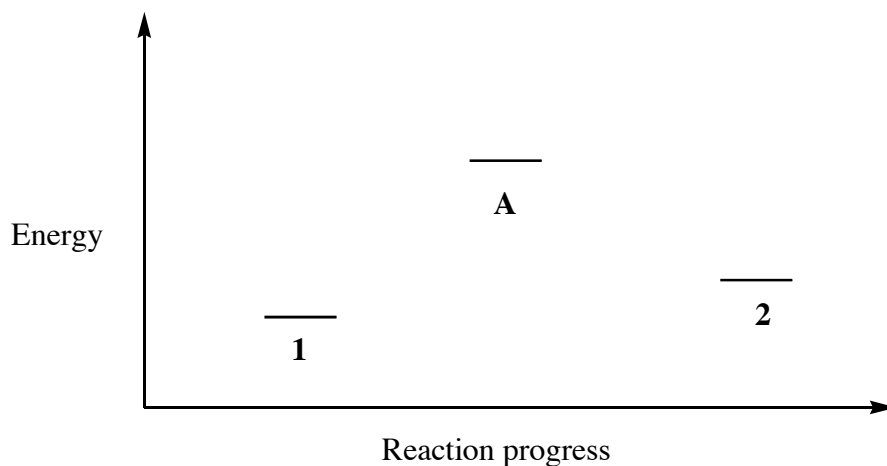
5c. Treatment of halides **1** or **2** with magnesium metal in ether produces allylic anion salt **B**, depicted as a resonance hydrid:

Draw the individual resonance forms that contribute to resonance hybrid **B**, and indicate which is the major and which is (are) the minor resonance forms. Give a rationale for your assignment, discussing the relative stabilities of the resonance forms you have drawn. (5 pts)

6. (Bonus) Draw the two chair forms for *cis*-1-bromo-3-ethylcyclohexane and for *trans*-1-bromo-3-ethylcyclohexane, estimate the energy difference between the conformers, show the relative percentages of each conformer present at equilibrium, circle the more stable conformer of each pair, and indicate which is more stable, the *cis* or the *trans* isomer.(10 points)

Congratulations!
Score:

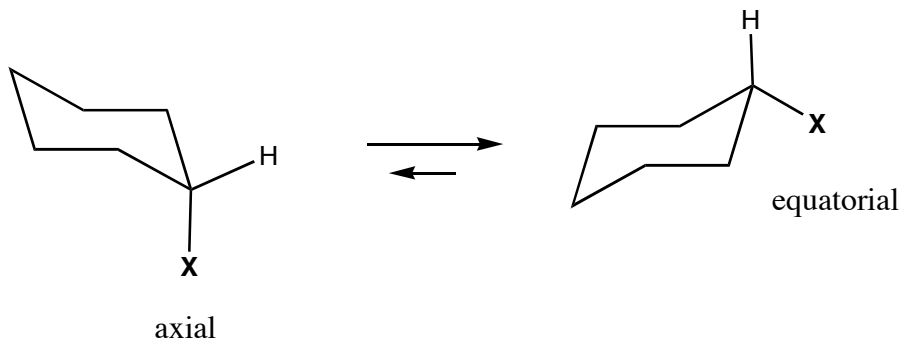1. _____ /10
2. _____ /20
3. _____ /20
4. _____ /25
5. _____ /25
Bonus:_____ /10
Total: _____ /100

Energy differences Between Axial and Equatorial Conformations in Monosubtsituted Cyclohexanes

axial

equatorial

X	E(axial)-E(equatorial)
-F	0.2 kcal/mol (0.8 kJ/mol)
-CN	0.2 kcal/mol (0.8 kJ/mol)
-Cl	0.5 kcal/mol (2.1 kJ/mol)
-Br	0.6 kcal/mol (2.5 kJ/mol)
-OH	1.0 kcal/mol (4.1 kJ/mol)
-COOH	1.4 kcal/mol (5.9 kJ/mol)
$-CH_3$	1.7 kcal/mol (7.1 kJ/mol)
$-CH_2CH_3$	1.8 kcal/mol (7.5 kJ/mol)
$-CH(CH_3)_2$	2.1 kcal/mol (8.8 kJ/mol)
$-C(CH_3)_3$	5.4 kcal/mol (23 kJ/mol)

The relationship between stability and isomer percentages at equilibrium

More stable isomer(%)	Less stable isomer (%)	Energy difference at 25°C
50	50	0 kcal/mol (0 kJ/mol)
75	25	0.651 kcal/mol (2.72 kJ/mol)
90	10	1.302 kcal/mol (5.45 kJ/mol)
95	5	1.744 kcal/mol (7.29 kJ/mol)
99	1	2.500 kcal/mol (11.38 kJ/mol
99.9	0.1	4.092 kcal/mol (17.11 kJ/mol