

Please print:

Last name: Answer Key

First name: _____

Chem 2061 Exam 3

Fall 2005

Andy Aspaas, Instructor

Monday, November 7, 2005

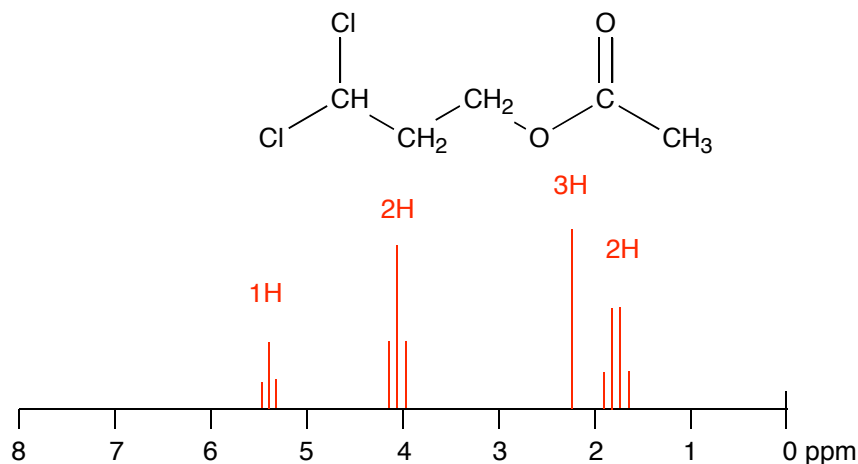
Instructions:

You have 55 minutes to complete this exam.

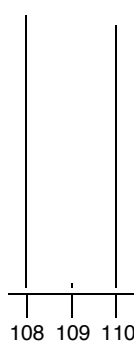
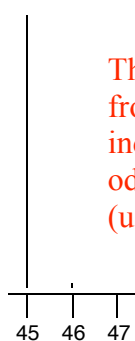
I, _____ have read and understand the directions given above, and pledge that I will follow all regulations with regard to Academic Dishonesty as outlined by this college when taking this exam.

Signature _____ Date and Time _____

1. Using the scale below, sketch the ^1H NMR spectrum for the following compound. Present the peaks with correct splitting patterns and at the approximate chemical shift (± 0.5 ppm). Just above each peak, indicate the relative integration value (e.g. "2H"). (16 pts)

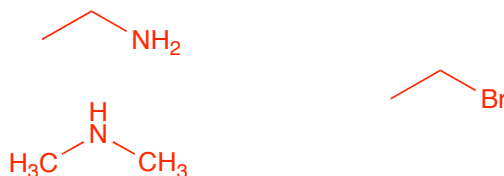


2. Below are molecular ion peaks from the mass spectra of two different compounds. Describe the recognizable traits of these peaks, and what those traits represent. (8 pts)

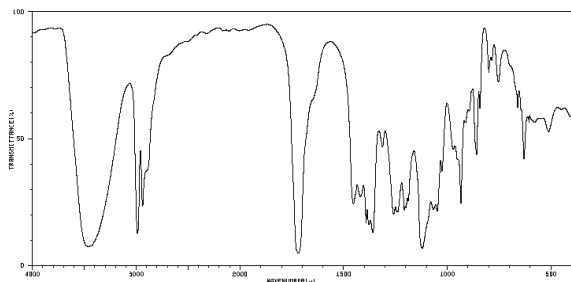


The molecular ion on the left comes from a compound with 7 hydrogens in its formula, and the one on the right comes from a compound with 5 hydrogens in its formula. Draw a structure that is consistent with one of these two molecular ions. (6 pts)

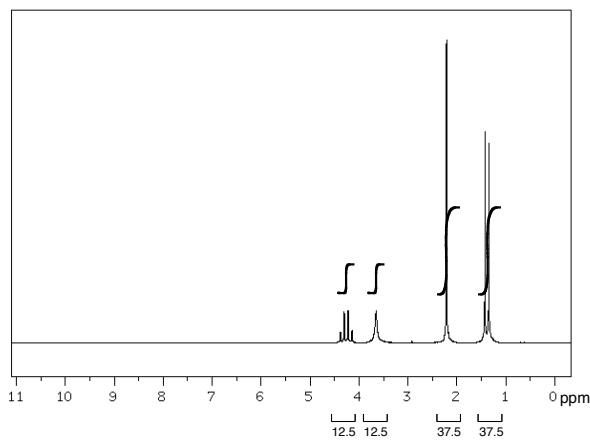
There's only enough mass for 2 carbons in either of the compounds.



3. Draw the structure of the molecule with the formula $C_4H_8O_2$ and the following IR and NMR spectra. Show all your work. (20 pts)

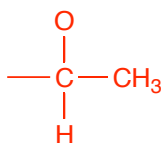


O-H str at $3200-3500\text{ cm}^{-1}$
 sp^3 C-H str below 3000 cm^{-1}
 isolated C=O at 1710 cm^{-1}

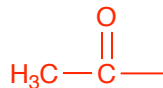


Peak ratios are 1:1:3:3
 1H quartet at 4.2 ppm
 1H broad singlet at 3.6 ppm
 3H singlet at 2.1 ppm
 3H doublet at 1.4 ppm

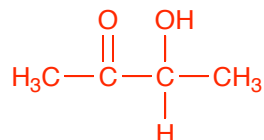
The 1H quartet at 4.2 ppm must be a methine next to a methyl *and* attached to an oxygen (there are no halogens in the formula). So, the 3H doublet must be that methyl group next to the methine. That gives us this fragment:



The broad singlet is most likely an OH hydrogen, since we see an OH stretch is present in the IR. The 3H singlet must be a methyl group with no hydrogens on adjacent carbons. Its chemical shift is consistent with hydrogens adjacent to a carbonyl, which we know is present from the IR. That makes this fragment:



That makes all the carbons and oxygens in the formula. So, the OH must be what's attached to the methine. Then there is only one way to put the pieces together:



4. For the following pairs of reaction conditions, circle the conditions that would react faster in an S_N2 reaction, and briefly explain why (just a few words). (12 pts)



S^- is a stronger nucleophile than OH^- because S is larger and more polarizable.

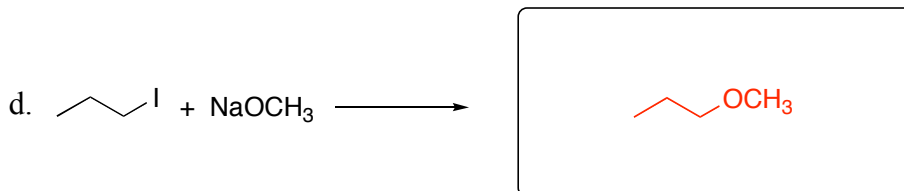
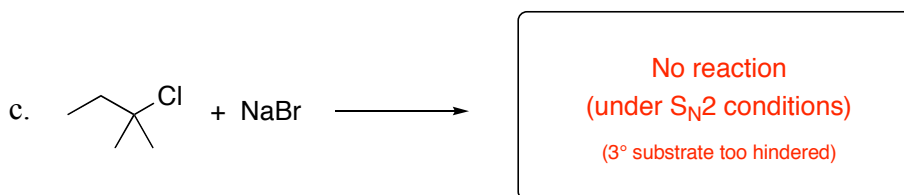
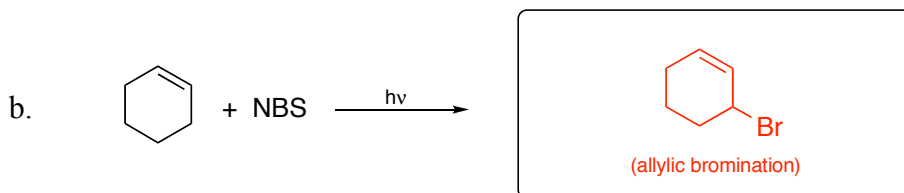
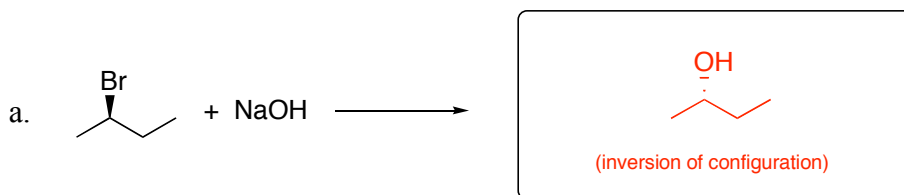


OH^- only becomes an acceptable leaving group when it is protonated, allowing a neutral water molecule to be ejected.

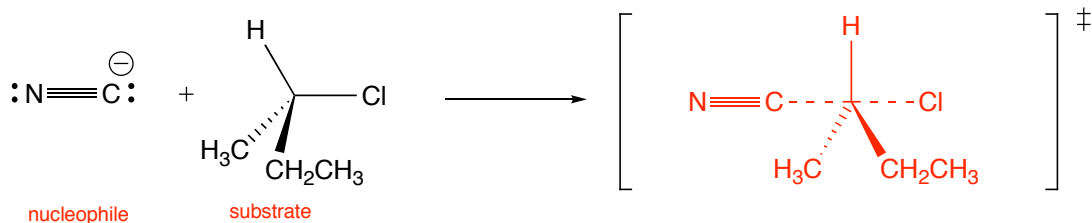


The primary chloride is less hindered and more easily attacked by the nucleophile than the secondary chloride.

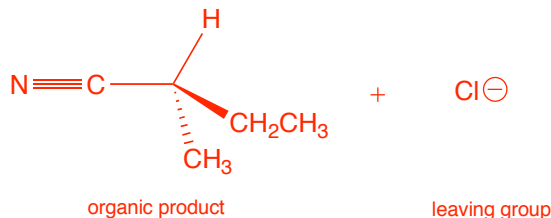
5. Predict the major organic product of the following reactions. Show the proper stereochemistry where appropriate. (16 pts)



6. a. The reactants shown below will undergo an S_N2 reaction. (10 pts)
- Draw the appropriate curved mechanism arrows for this reaction.
 - Label the nucleophile and substrate.
 - Draw the transition state of the reaction, with correct geometry.



- b. Draw the products of this reaction, with correct stereochemistry. Label the organic product and leaving group. (10 pts)



IR Stretching frequencies (cm^{-1})

- 3300 alcohol O–H (broad)
 amine N–H (broad with spikes)
 alkyne sp^3 C–H
- 3000 alkene sp^2 C–H (just above 3000)
 alkane sp^3 C–H (just below 3000)
 acid O–H (broad)
- 2200 nitrile C≡N (just above 2200)
 alkyne C≡C (just below 2200)
- 1710 carbonyl C=O (esters higher, conjugated and amides lower)
- 1660 alkene C=C (conjugated lower, aromatic lower yet)

NMR Chemical Shifts (ppm)

