Chemistry Department

University of Alberta

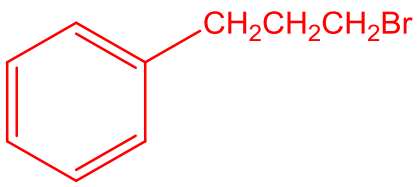
CHEM 263

Exam I

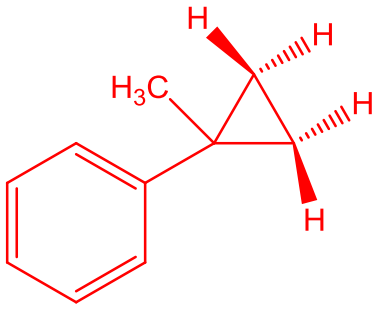
Friday, June 1, 2012

1. Give a structure consistent with each of the following sets of ^{1}H NMR data: (10 points)

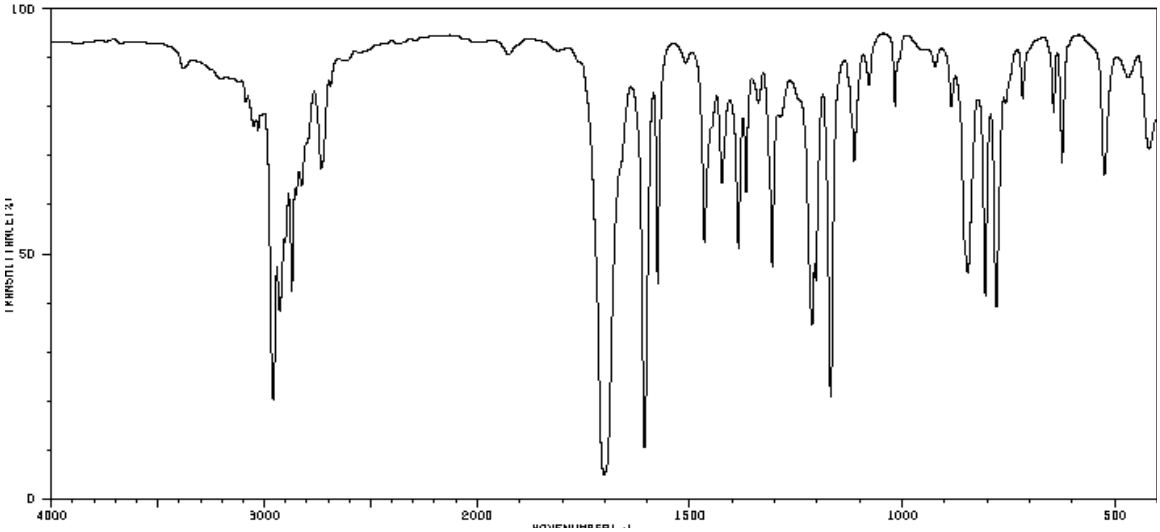
   a. $C_9H_{11}Br$ δ = 2.15 ppm (2H, quintet)
   δ = 2.75 ppm (2H, triplet)
   δ = 3.38 ppm (2H, triplet)
   δ = 7.22 ppm (5H, singlet)



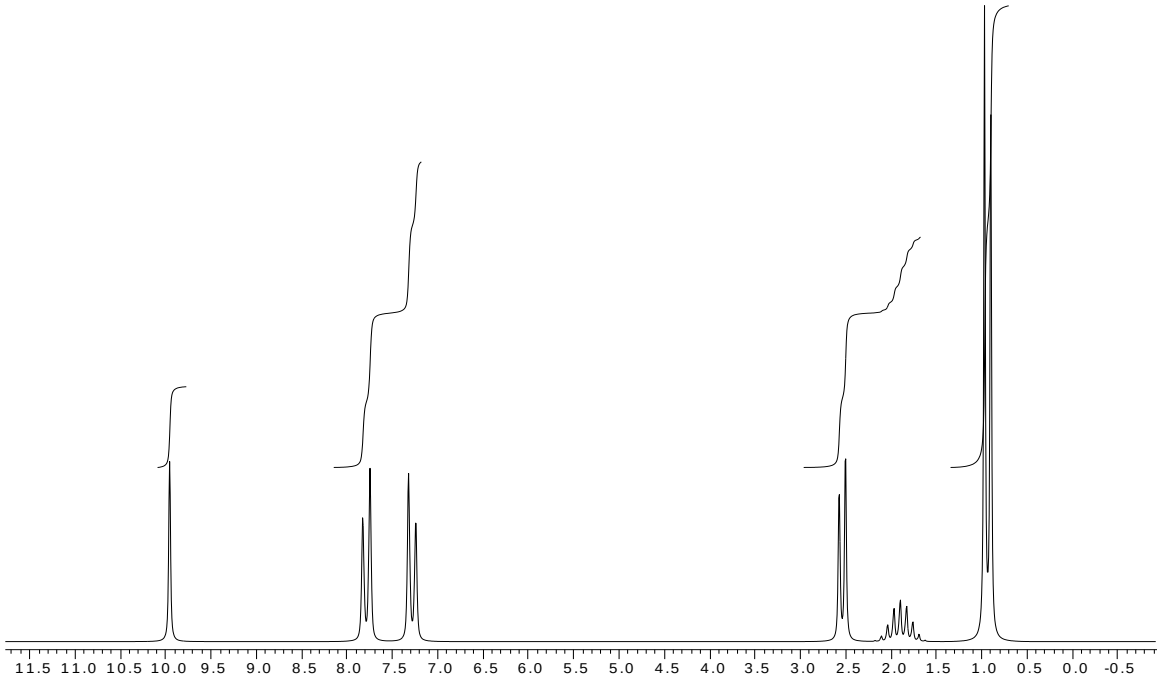
   b. $C_{10}H_{12}$ δ = 0.65 ppm (2H, multiplet)
   δ = 0.81 ppm (2H, multiplet)
   δ = 1.37 ppm (3H, singlet)
   δ = 7.17 ppm (5H, singlet)



2. The IR and ^{1}H NMR spectra of a compound of molecular formula $C_{11}H_{14}O$ are given below.



SDBSWeb : http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology, 29 May 2012)



a. Calculate the degree of unsaturation. (1 point)

(2 x 11 – 14 + 2)/2 = 5

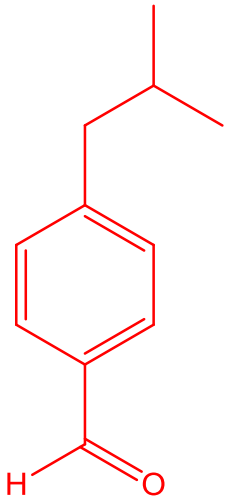
b. List the possible functional groups gleaned from the molecular formula. (2 points)

Alcohol
Aldehyde
Ether
Ketone
Phenol

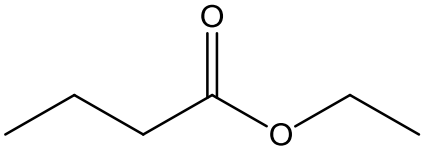
c. What is the functional group that the IR spectrum shows to be present in the unknown? (2 point)

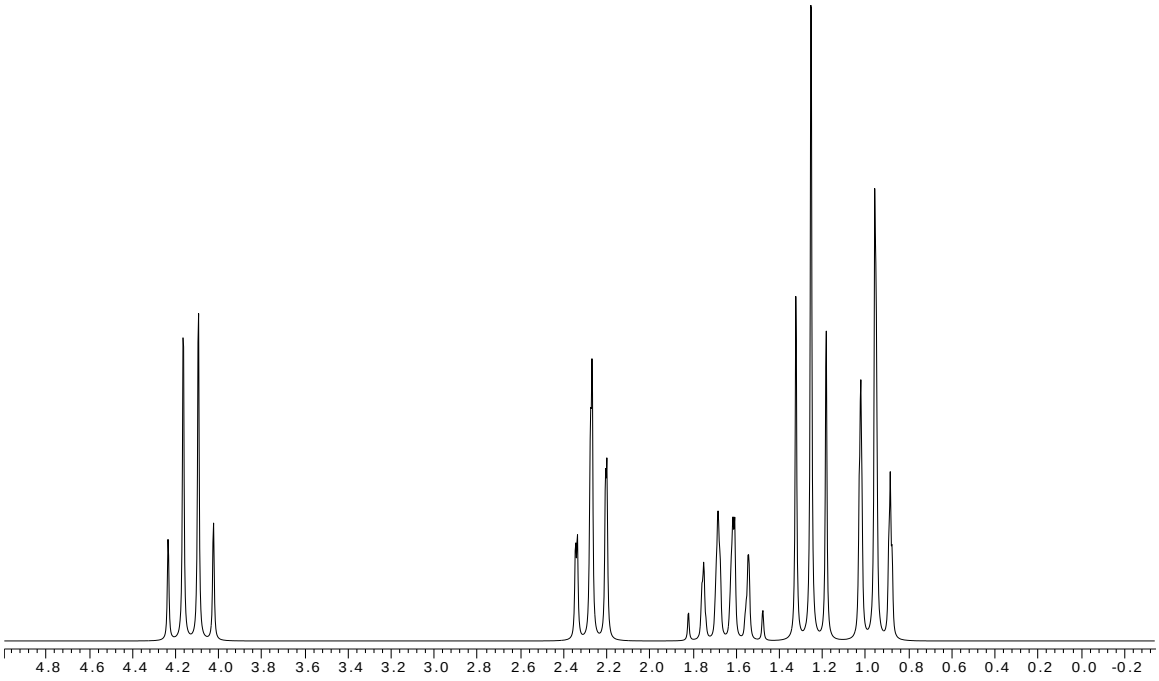
Aldehyde

d. Draw a table that lists chemical shifts and multiplicity. Then propose a structure for this compound. (10 points)

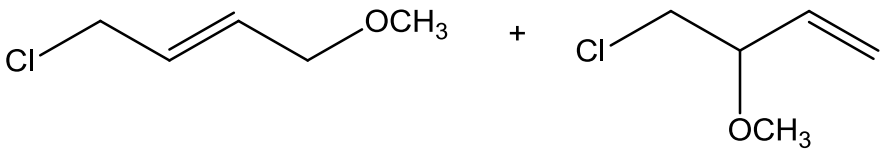


3. Sketch the expected ^{1}H NMR spectrum of the following compound: (10 points)

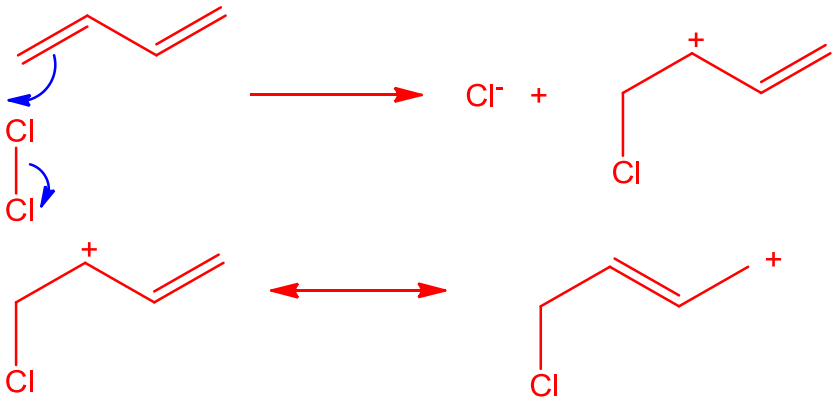


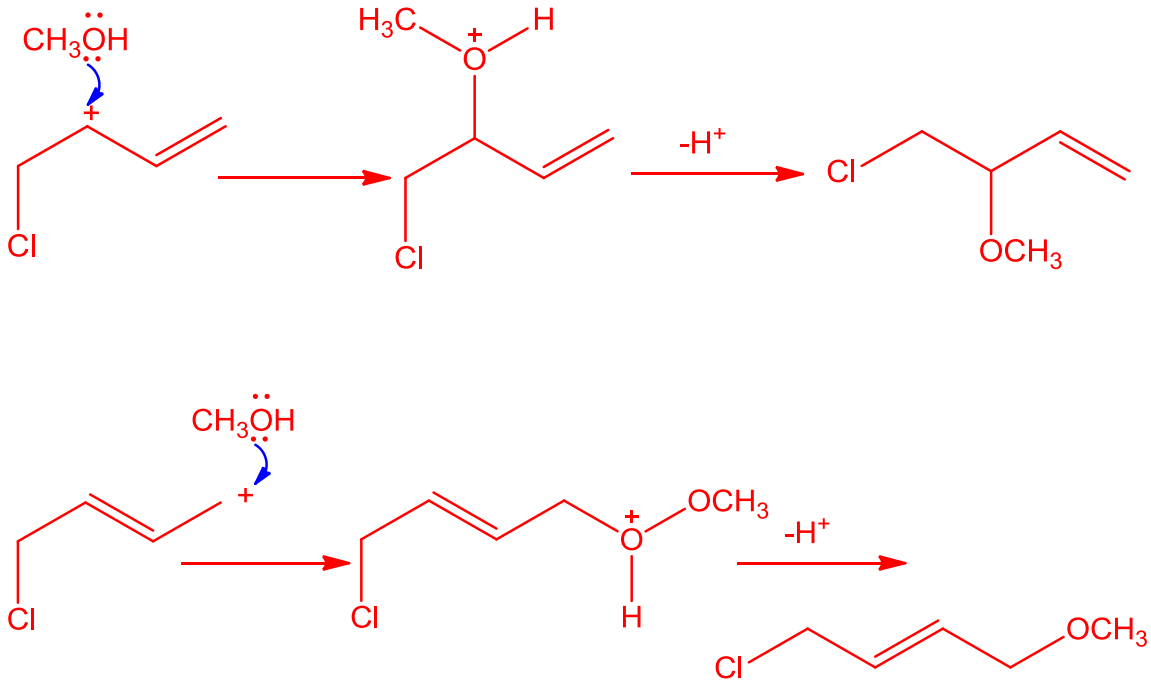


4. When a solution of 1,3-butadiene in CH_3OH is treated with chlorine, the products are:

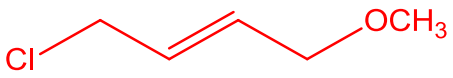


a. Propose a mechanism that accounts for their formation (don't forget the arrows). (10 points)

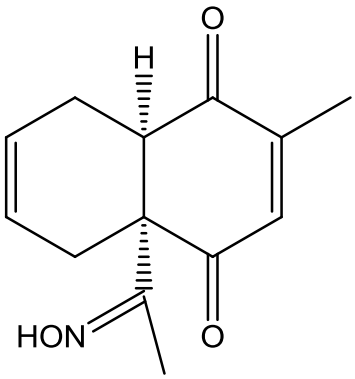




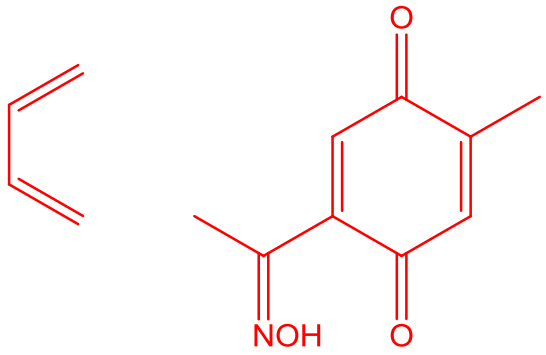
b. Which is the product of thermodynamic control. (2 points)



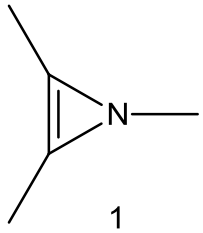
5. Tetrodotoxin is a poison isolated from the ovaries and liver of the puffer fish. One step in the synthesis of this toxin involves a Diels-Alder reaction to make the following compound:



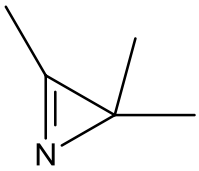
Draw the necessary diene and dienophile to synthesize this compound. (4 points)



6. Explain why azirines of structure 1 have never been isolated, whereas the isomeric azirines of structure 2 are well known. (6 points)



1



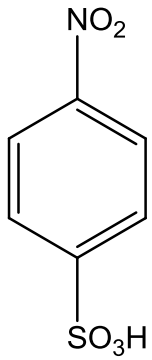
2

Both are cyclic and planar.

Structure 2 is not conjugated – there is a ring carbon bonded to four other atoms.

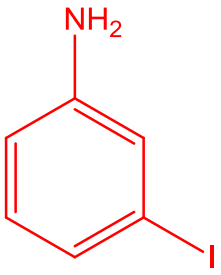
Structure 1 is conjugated as the lone pair is in a p orbital thus there are 4 π electrons and thus the ring is antiaromatic

7. Name the following compound: (2 points)



p-nitrobenzenesulfonic acid or 4-nitrobenzenesulfonic acid

8. Draw the structure of *m*-iodoaniline. (2 points)



9. Provide a synthetic pathway for the following transformation: (6 points)