

Chemistry Department

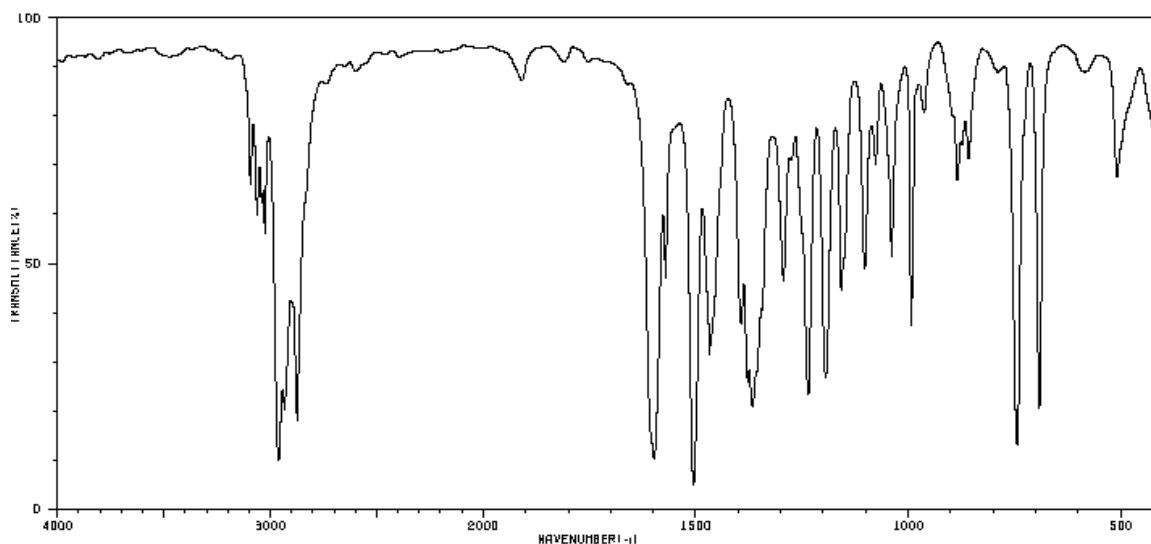
University of Alberta

CHEM 263

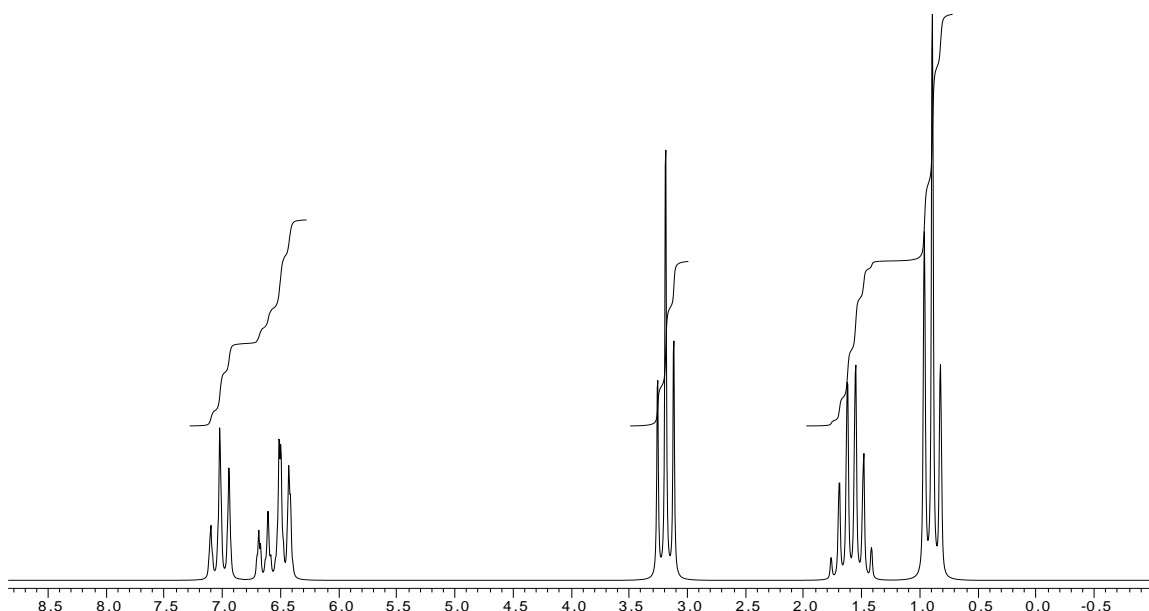
Exam I

Friday, June 3, 2011

1. The IR and ^1H NMR spectra of a compound of molecular formula $\text{C}_{12}\text{H}_{19}\text{N}$ are given below.



SDBSWeb : <http://riodb01.ibase.aist.go.jp/sdbs/> (National Institute of Advanced Industrial Science and Technology, 30 May 2011)



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

$$(2 \times 12 + 1 - 19 + 2) / 2 = 4$$

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

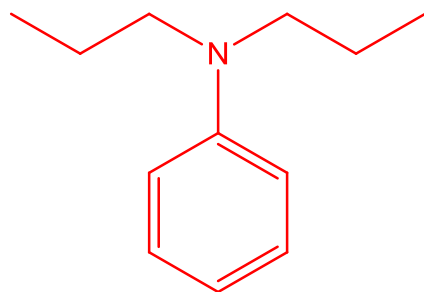
primary amine, secondary amine, tertiary amine, nitrile

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

tertiary amine

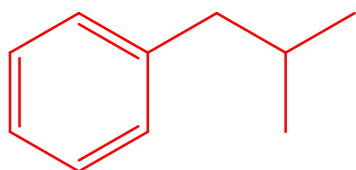
- d. Draw a table that lists chemical shifts and multiplicity. Then propose a structure for this compound. (10 points)

δ (ppm)	multiplicity	neighbours	# hydrogens	origin
6.5 - 7	m		5	Monosubstituted benzene
3.2	t	2	4	-CH ₂ - attached to N
1.6	6 peaks	5	4	-CH ₂ - attached to CH ₃ and -CH ₂ -
0.9	t	2	6	CH ₃

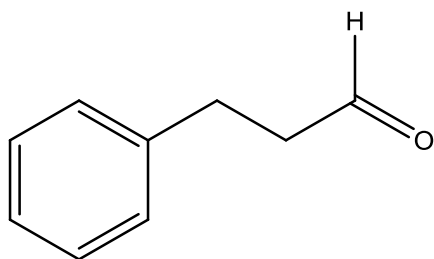


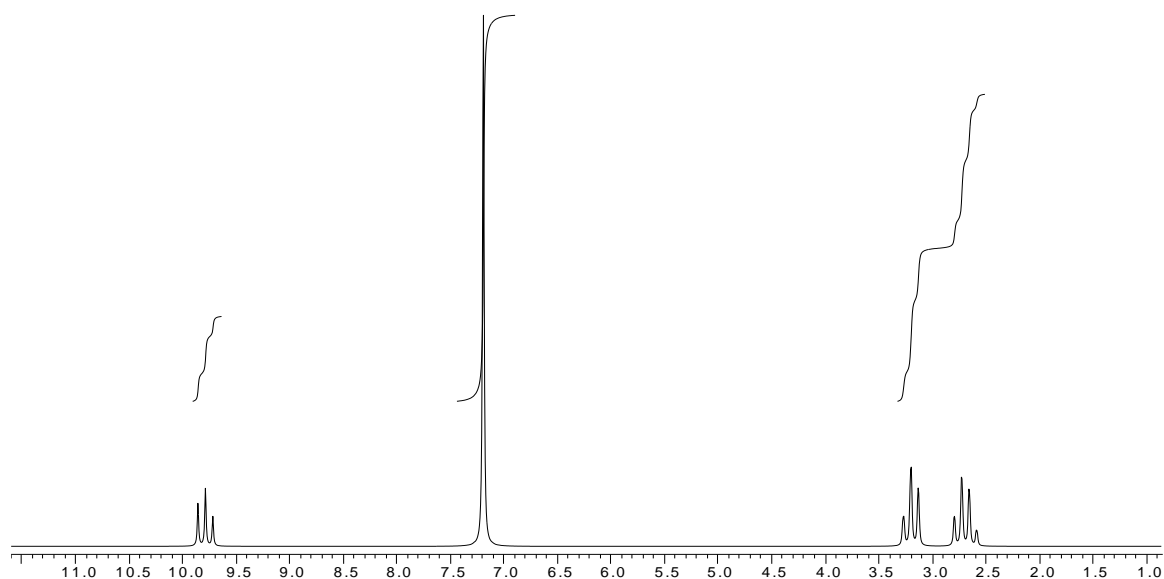
2. Propose a structure for the compound that fits the following data: (5 points)

$C_{10}H_{14}$ $\delta = 0.88$ ppm (6H, doublet)
 $\delta = 1.86$ ppm (1H, multiplet)
 $\delta = 2.45$ ppm (2H, doublet)
 $\delta = 7.12$ ppm (5H, singlet)

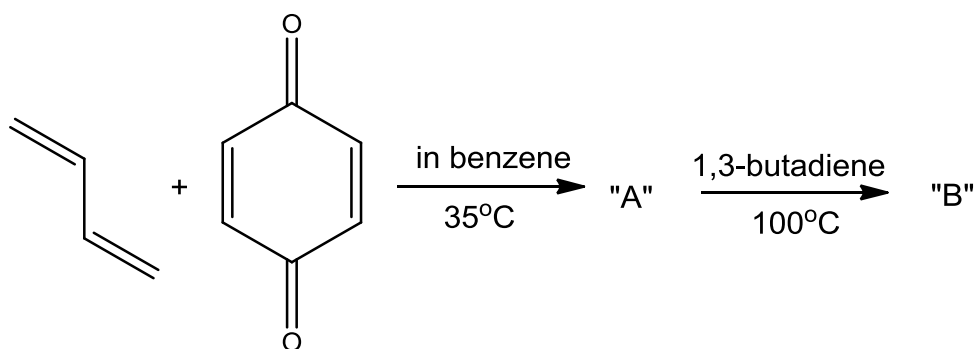


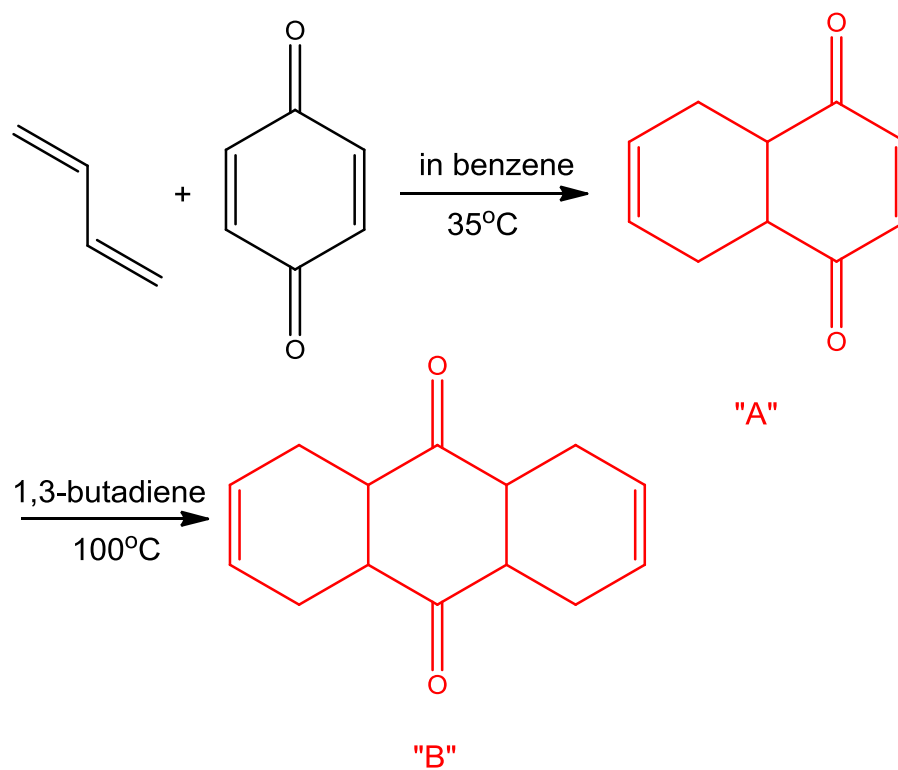
3. Sketch the expected 1H NMR spectrum of the following compound: (10 points)



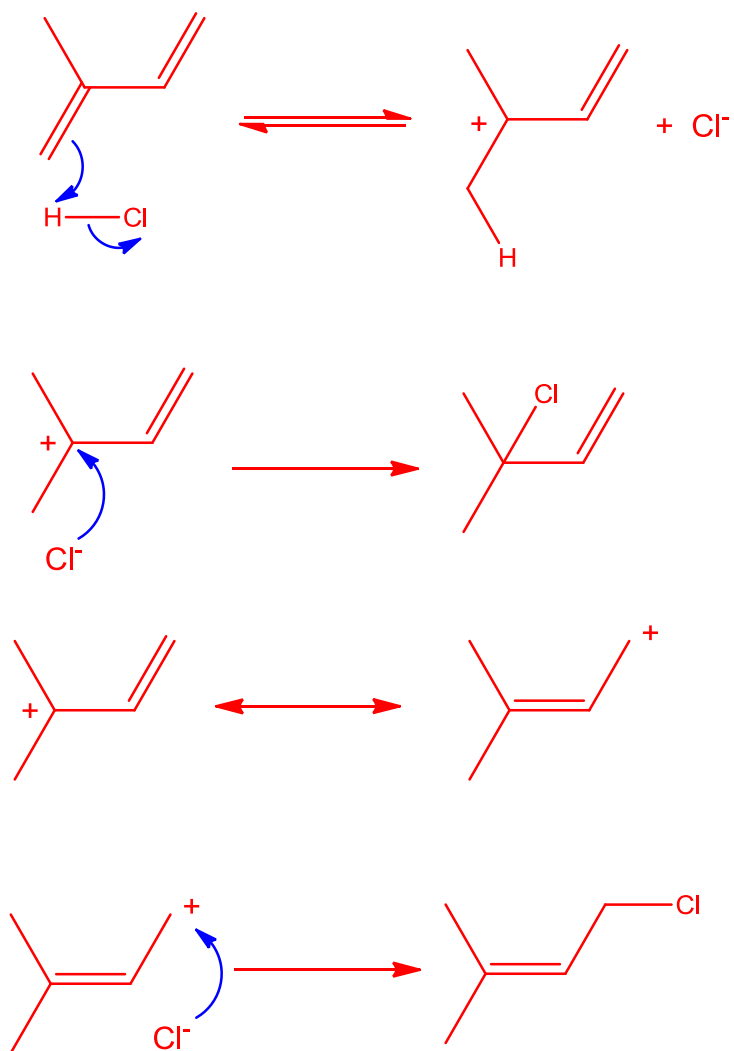


4. Draw the structures of compounds "A" and "B" in the following reaction sequence: (6 points)

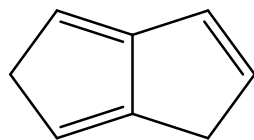




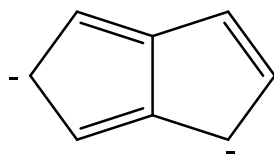
5. 2-methyl-1,3-butadiene reacts with HCl to yield only 3-chloro-3-methyl-1-butene and 1-chloro-3-methyl-2-butene. Explain by means of a mechanism. (8 points)



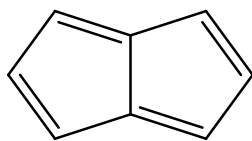
6. The following triene can be readily deprotonated twice:



and a stable dianion is formed:



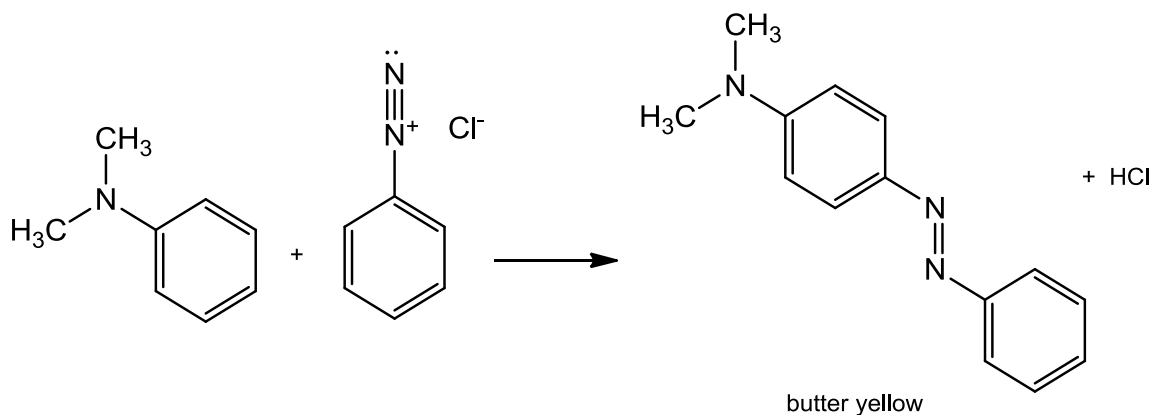
However the neutral analog of the dianion, the following tetraene, is extremely unstable:



Explain. (6 points)

Both are cyclic, planar, and have the π electrons delocalised over the ring. However the anion has a Hückel number of π electrons, 10, and is aromatic whereas the tetraene has 8 and so is antiaromatic.

7. Butter yellow is a dye that was used to colour margarine. However it has been found to be carcinogenic and therefore is no longer permitted in the food industry. The dye can be made by the following reaction:

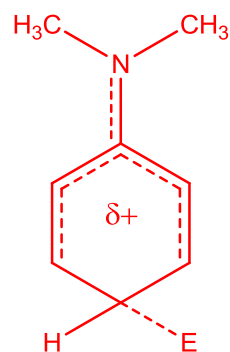


- a. Is this an example of electrophilic aromatic substitution? (1 point)

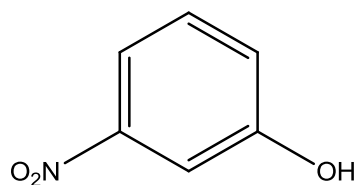
Yes

- b. Explain how the $(\text{CH}_3)_2\text{N}-$ group activates the ring. Use "E" to represent the electrophile. (3 points)

The N stabilizes the transition state for the rate determining step of the reaction by electron donation through the resonance effect.

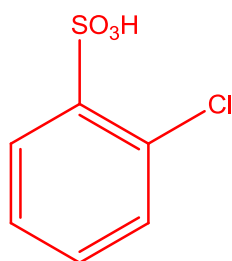


8. Name the following compound: (2 points)



m-nitrophenol or 3-nitrophenol

9. Draw the structure of *o*-chlorobenzenesulfonic acid. (2 points)



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

