

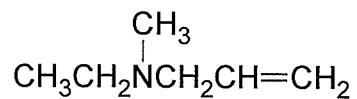
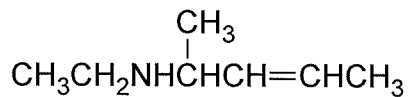
Organic Chemistry 212
Problem Set 1
Spring 2018

Name:

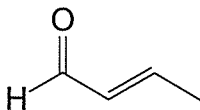
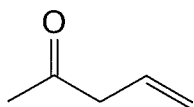
Answer the following:

1) How would you distinguish between the following pairs of compounds with IR:

a)



b)



2) Give a plausible structure from the following MS:

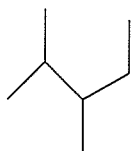
3) A compound (C_4H_6) has two signals of approximately equal intensity in its ^{13}C NMR spectrum; one is a CH_2 carbon at 30.2 ppm, the other a CH at 136 ppm. Identify the compound.

4) A compound with the molecular formula $C_6H_{10}O_2$ gives a 1H NMR spectrum consisting of two singlets. The singlet at 2.2 ppm integrates to 6H. The other at 2.7 ppm integrates to 4H. What is the structure of the compound?

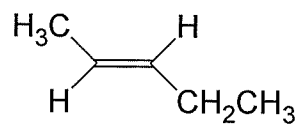
Answer the following questions dealing with spectroscopy.

For each compound, give the expected splitting patterns for each nonequivalent proton:

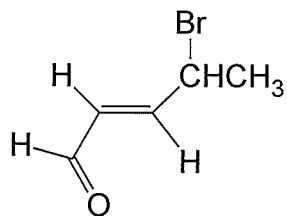
1)



2)



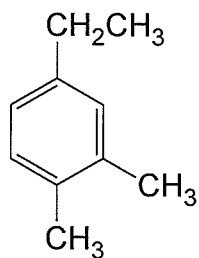
3)



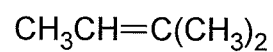
For question 2, show the tree diagram for each nonequivalent set of protons. Then, sketch the proton NMR.

How many peaks would you expect in the proton-noise decoupled ^{13}C NMR for each compound.

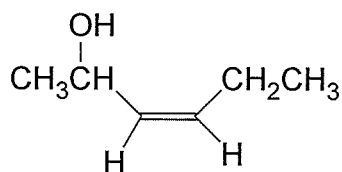
1)



2)



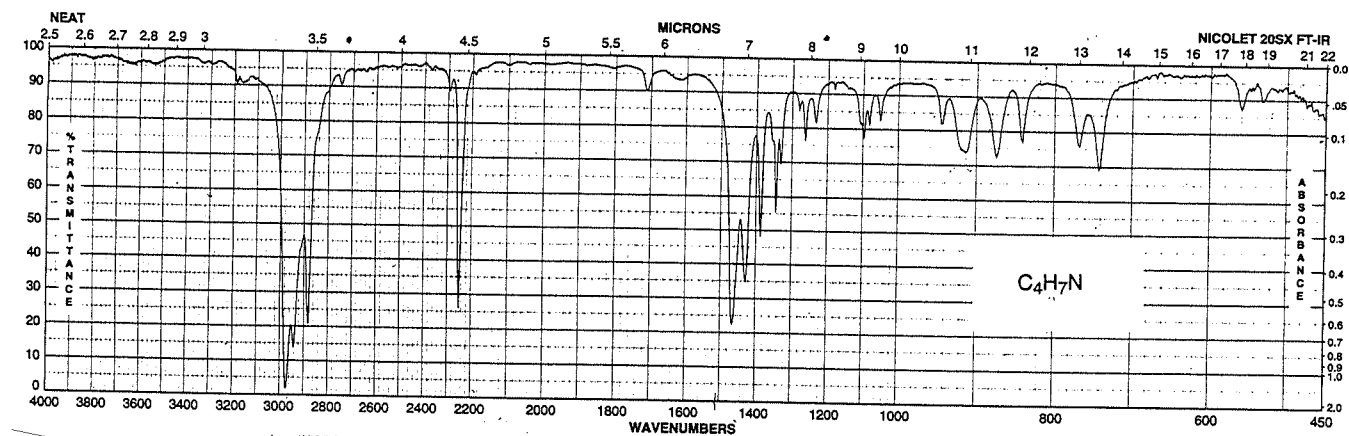
3)



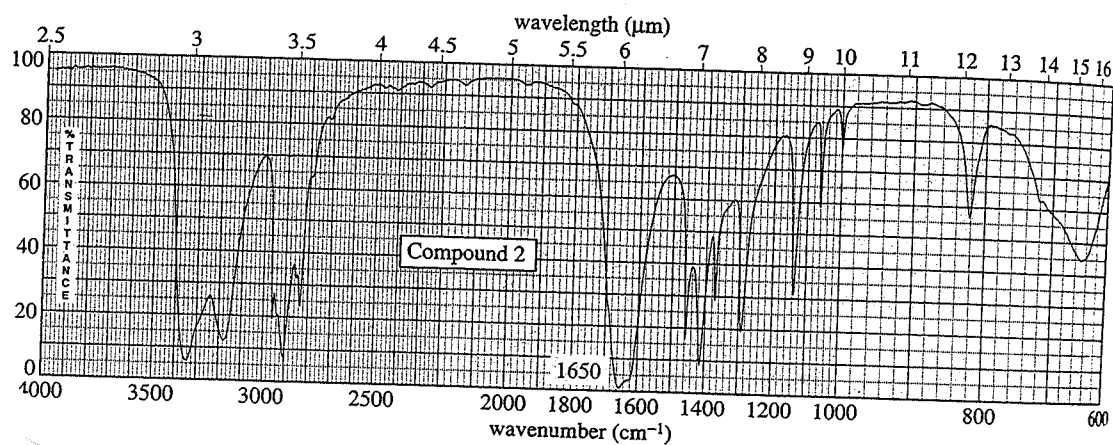
For question 3, give the splitting expected for each nonequivalent carbon in the off resonance mode.

Using the molecular formula and the IR, give the structure represented in each case ().

1) C_4H_7N



2) $C_5H_{11}NO$



Give the structure of each of the following compounds on the basis of their ^1H NMR spectra and molecular formula.

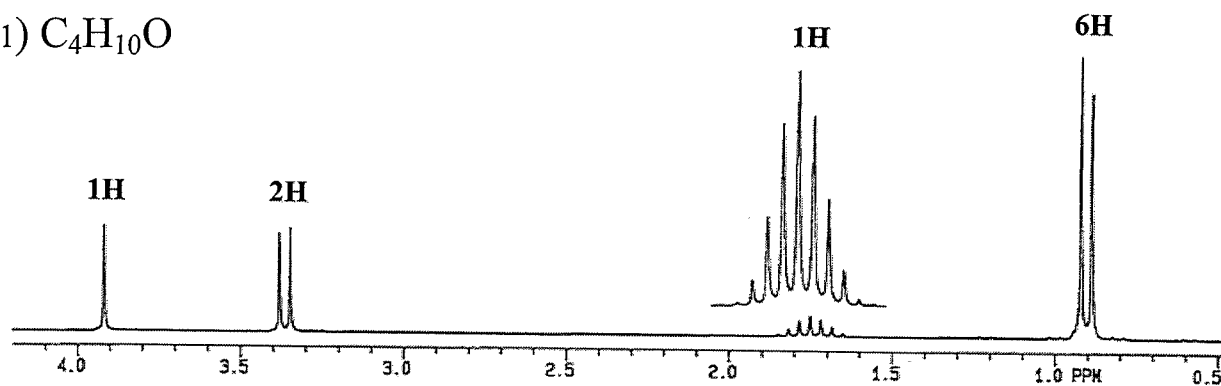
1) $\text{C}_4\text{H}_8\text{O}_3$ 1.27 ppm (triplet, 3H)
 3.66 ppm (quartet, 2H)
 4.13 ppm (singlet, 2H)
 10.9 ppm (singlet, 1H)

2) $\text{C}_4\text{H}_6\text{Cl}_2$ 2.2 ppm (singlet, 3H)
 4.1 ppm (doublet, 2H)
 5.7 ppm (triplet, 1H)

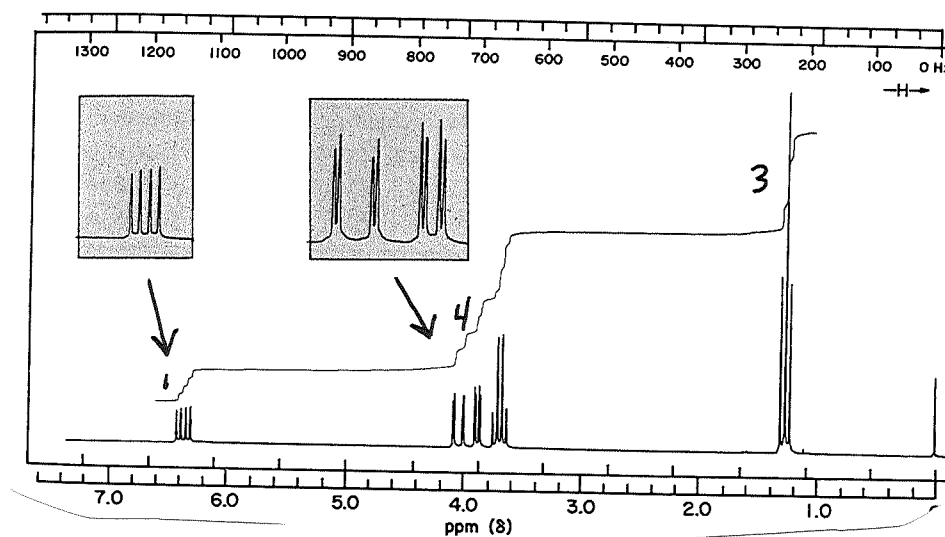
3) C_6H_{12} 0.9 ppm (triplet, 3H)
 1.6 ppm (singlet, 3H)
 1.7 ppm (singlet, 3H)
 2.0 ppm (quintet, 2H)
 5.1 ppm (triplet, 1H)

Propose the structure for each compound from the following spectra ():

1) $C_4H_{10}O$

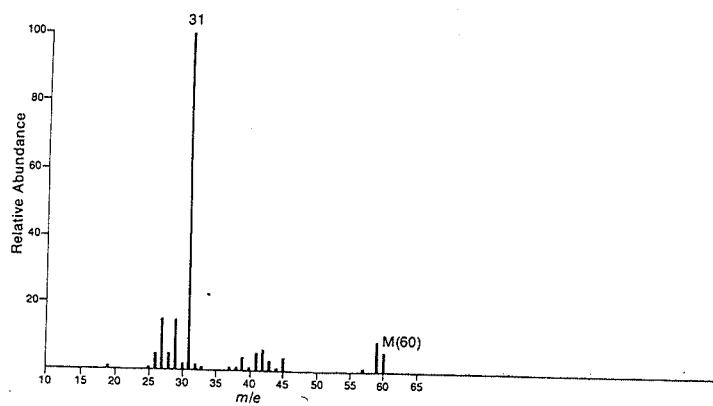


2) C_4H_8O

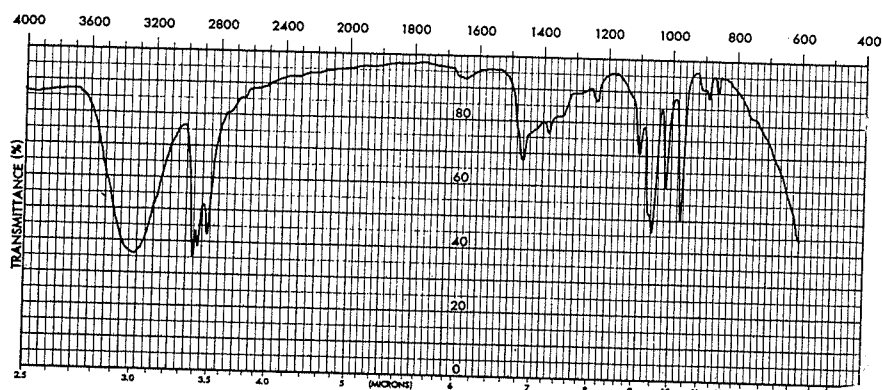


Give the structure of each compound based on the following combined spectra ():

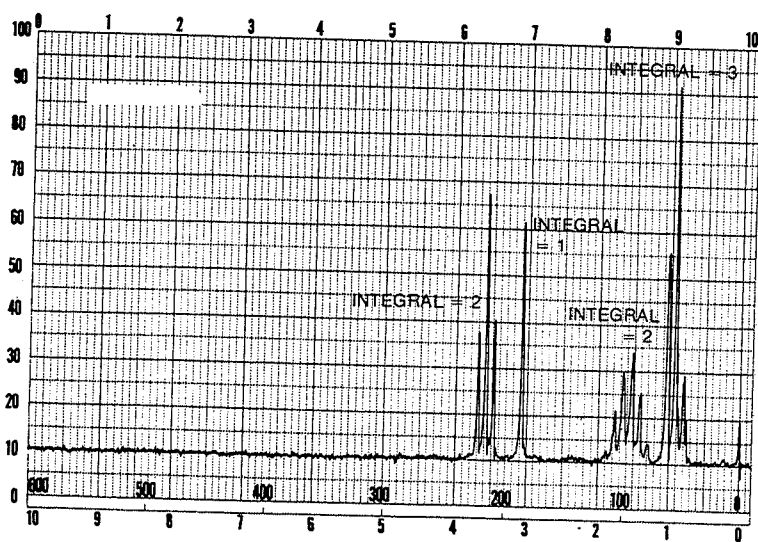
1)



MASS SPECTRUM

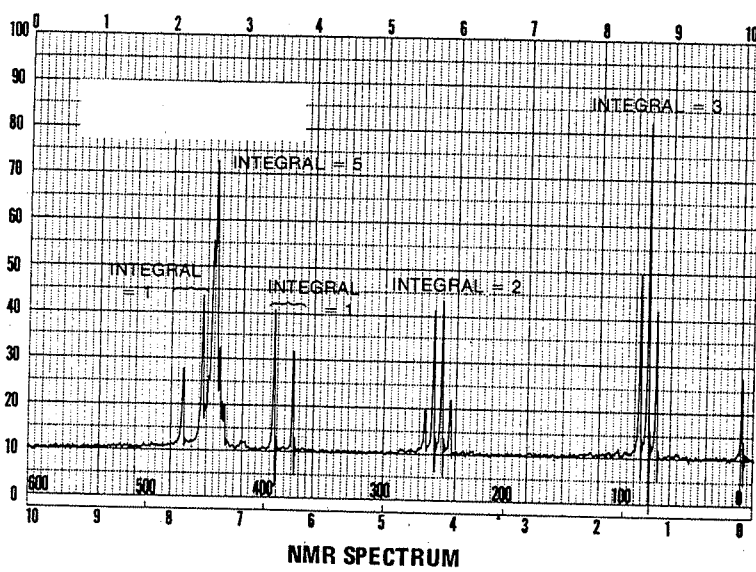
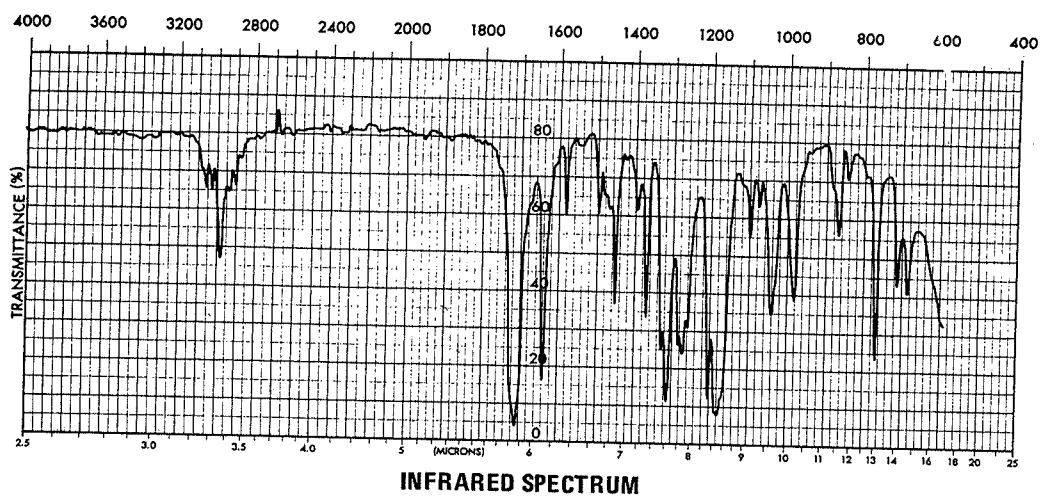


INFRARED SPECTRUM



NMR SPECTRUM

2) $C_{11}H_{12}O_2$



Answer the following ():

3-Bromo-2,3-dimethylpentane was treated with KOH in refluxing ethanol. The resulting alkene mixture was separated using preparative GC into four fractions. The principal product was found by proton NMR to be 2,3-dimethyl-2-pentene. A second product was found to be 2-ethyl-3-methyl-1-butene. The remaining two products had the following ^{13}C NMR chemical shifts:

Isomer 3: 12.4, 17.8, 20.6, 28.5, 117.9, and 141 ppm

Isomer 4: 13.0, 13.1, 21.6, 37.4, 116.2, and 141.5 ppm

What are the structures for ALL four isomers?