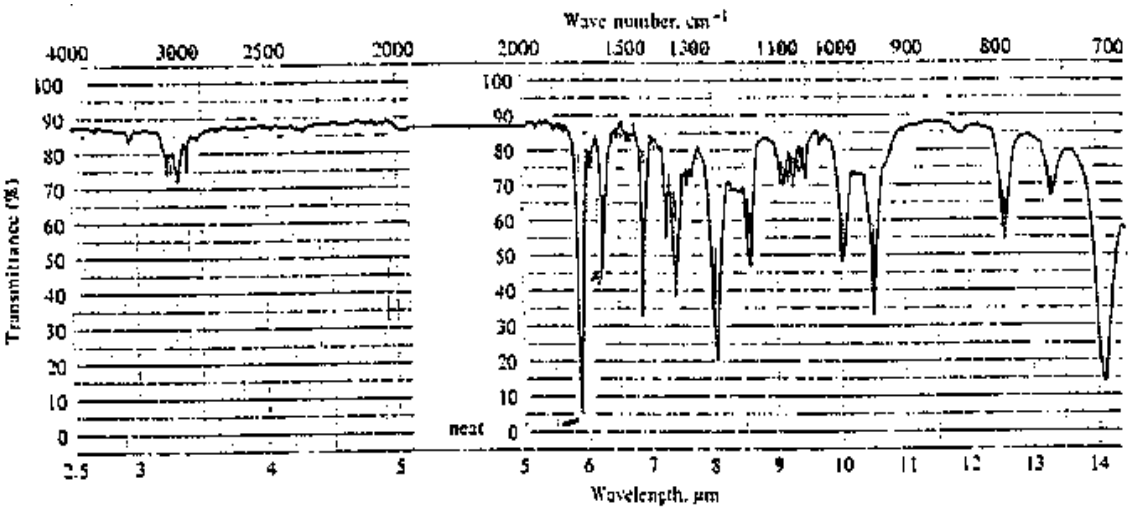
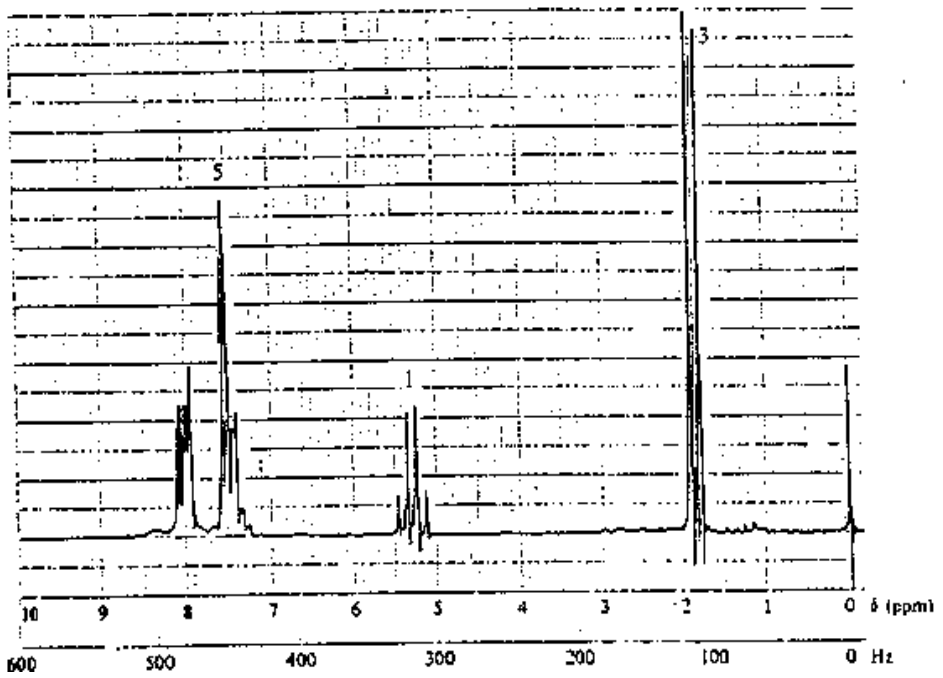
Spectroscopy Problems
In-class and Homework

The following are problems in determining compound structure form NMR and sometimes IR spectra. We will cover some of them in class and additional examples are included for your enjoyment...NOT!... The text does not include enough examples to get confident that you can solve such problems so use these for more practice. Additional problems can be found in the later chapters of the text. These are scanned in and some of the resolution leaves a lot to be desired. I will provide information as text along with the figures. Answers can be found in the Answers to spectroscopy file.

Problem 2.

Integration values left to right are: 5 for both peaks at 7-8 ppm, 1, 3
Splitting is multiplet, multiplet, quartet, doublet
Formula is C_9H_9OBr





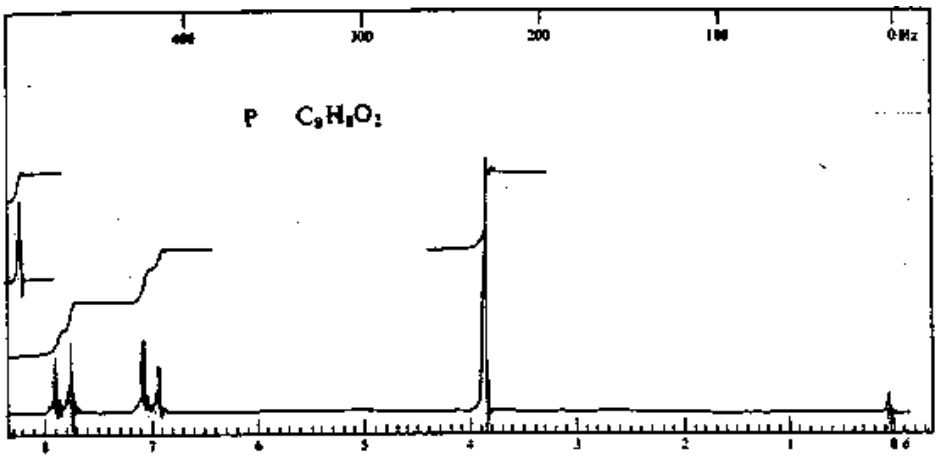
C_9H_9OBr

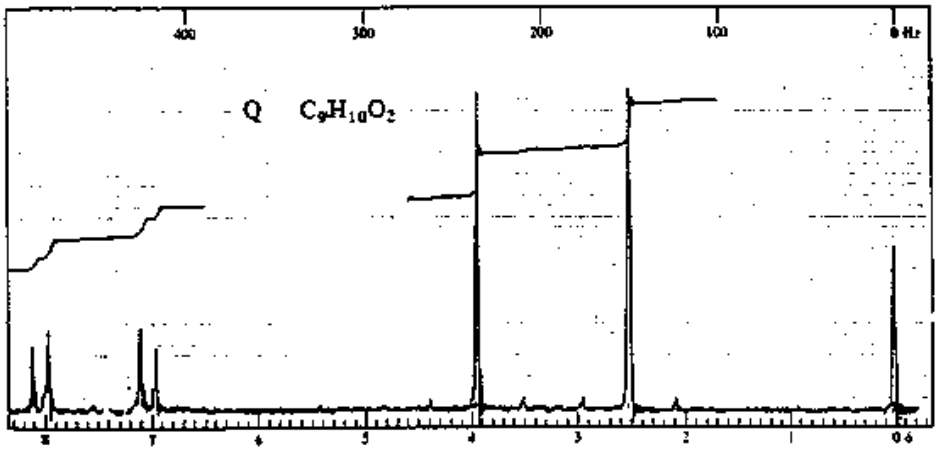
Problem 1

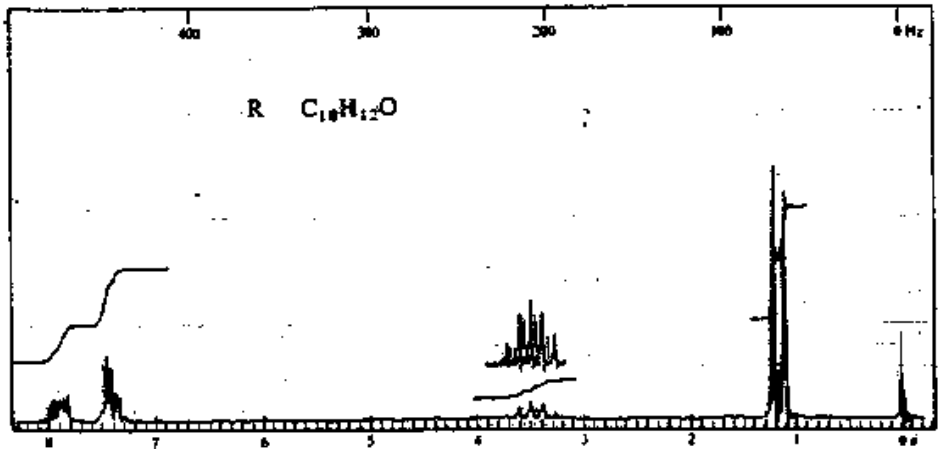
P. Integrator heights in arbitrary units: low field to high- 2.1, 4.0, 3.9, 6.2
Splitting: singlet (offset from 10-11 ppm), doublet, doublet singlet
Formula is $C_8H_8O_2$

Q. Integrator height is: 2.5, 2.5, 4, 4
Splitting is doublet, doublet, singlet, singlet
Formula is $C_9H_{10}O_2$

R Integrator height is: 4.1, 6, 2.1, 11.9
Splitting is multiplet, multiplet, 5, doublet
Formula is $C_{10}H_{12}O$


P $C_9H_8O_2$


Q $C_9H_{10}O_2$

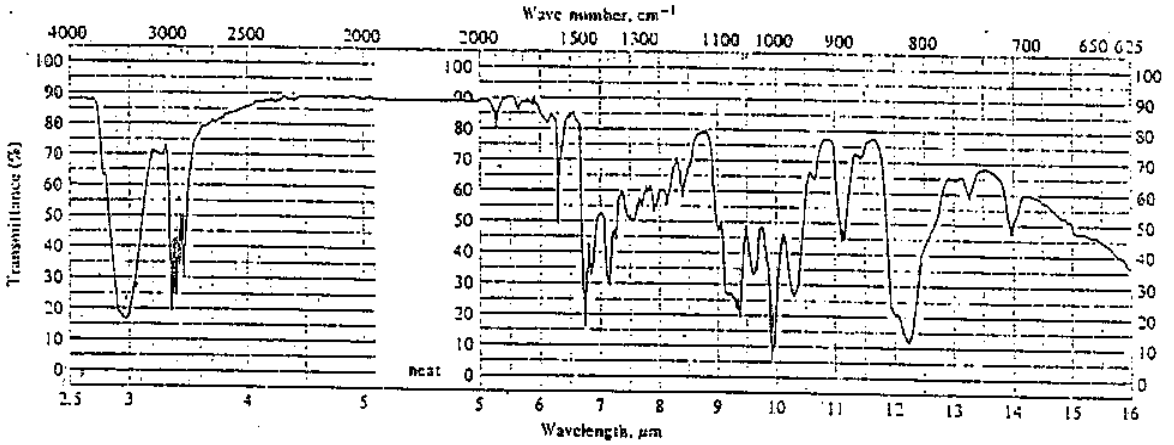

R $C_{10}H_{12}O$

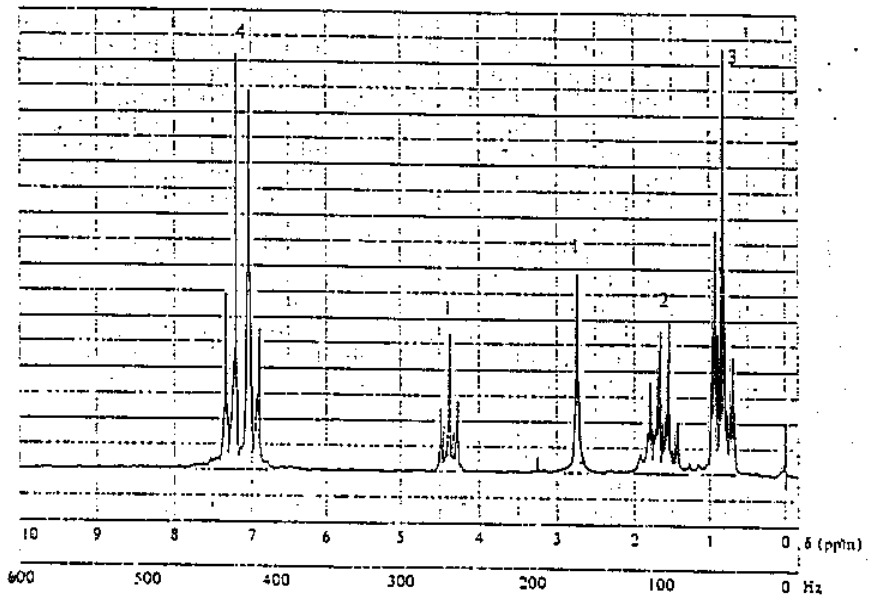
.Problem 3

Integration: 4, 1, 1, 2, 3

Splitting is quartet, triplet, singlet, 4 or 5, triplet

Formula is $C_9H_{11}BrO$





$C_9H_{11}BrO$

Problem 5.

SS Integration: 5, 2, 3

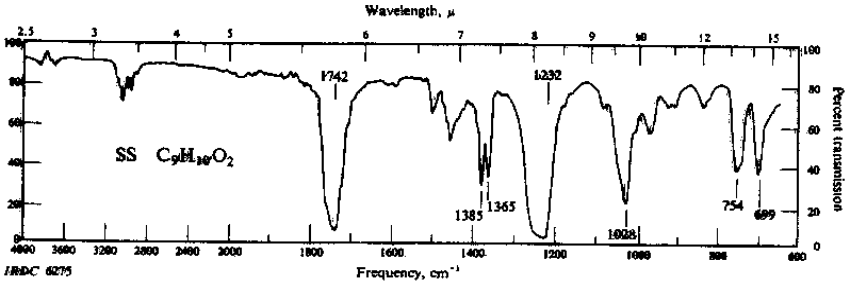
Splitting: all singlets

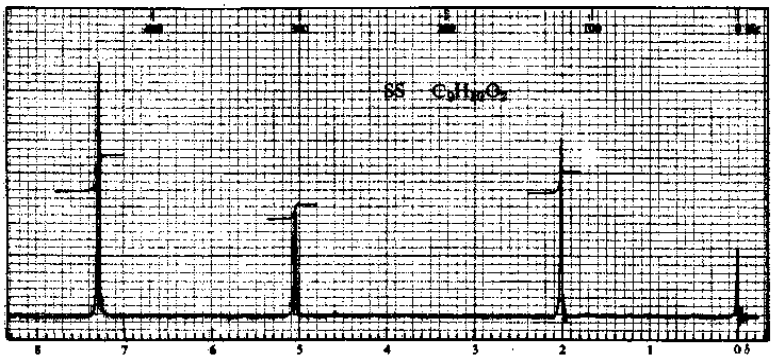
Formula = $C_9H_{10}O_2$

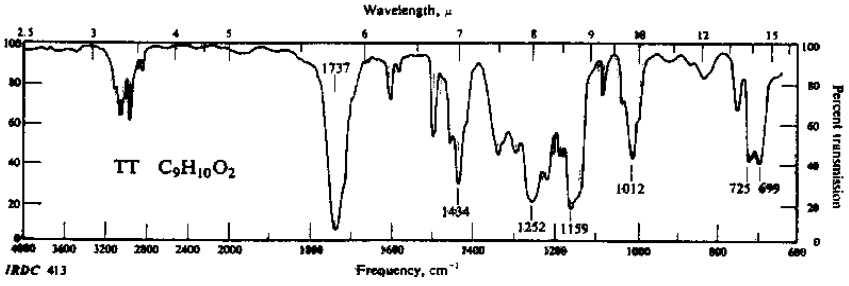
TT: Integration: 5, 5

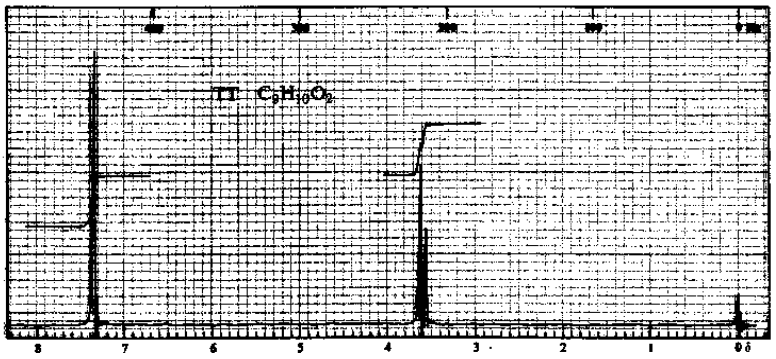
Splitting: singlet, doublet

Formula = $C_9H_{10}O_2$



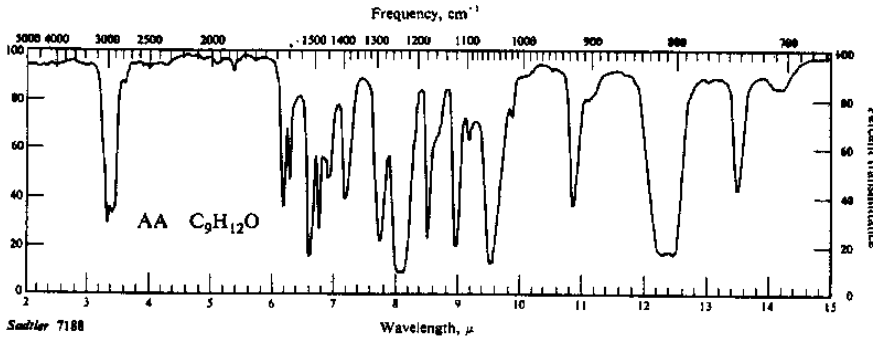


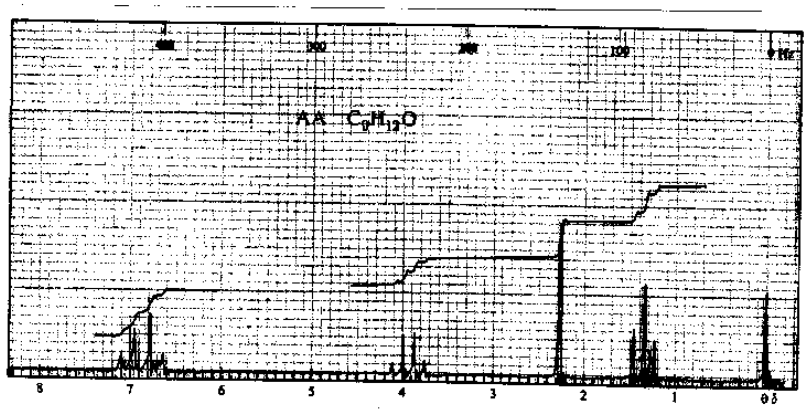


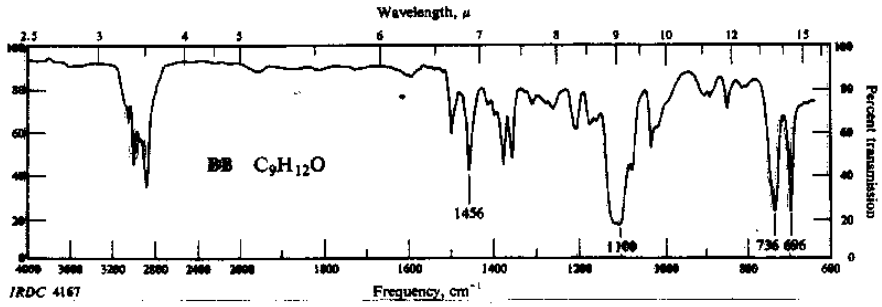


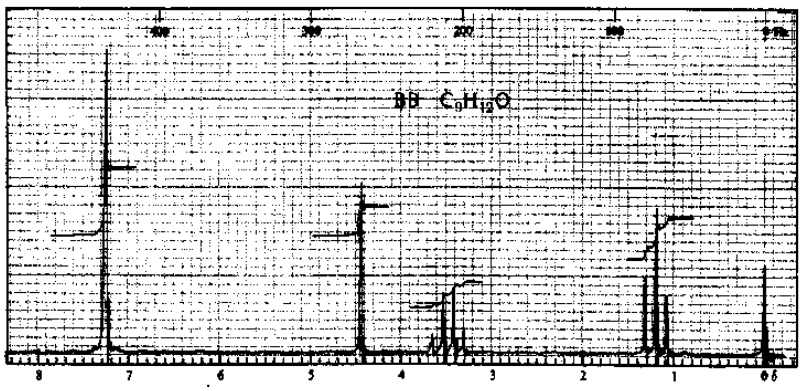
AA. Integration: 4, 2, 3, 3, Splitting; 4, 4, 1, 3 Formula = C9H12O

BB. Integration: 5, 2, 2, 3 Splitting: singlet, singlet, quartet, triplet Formula: $C_9H_{12}O$

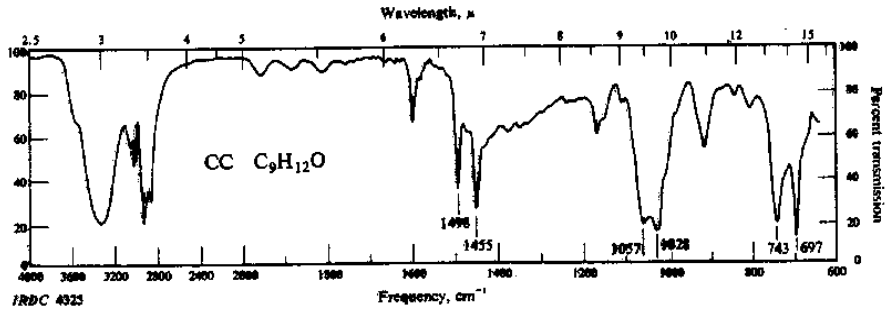








Problem 7



CC Integration: 5, 3, 2, 2

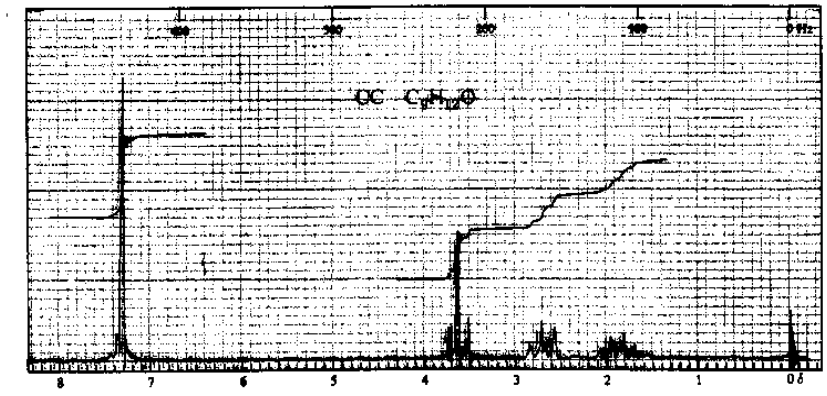
Splitting: singlet, triplet, triplet-quartet?, multiplet

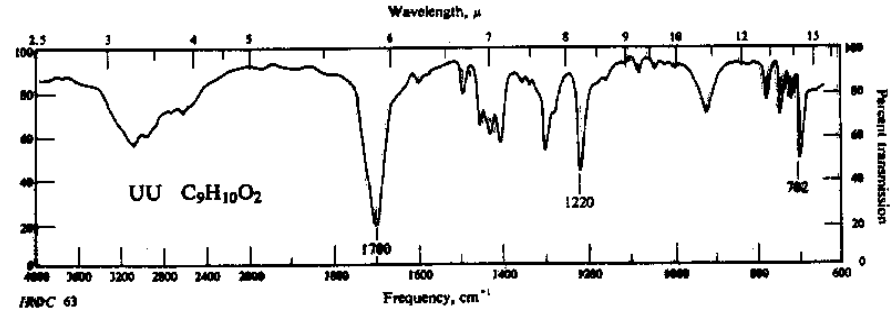
Formula: $C_9H_{12}O$

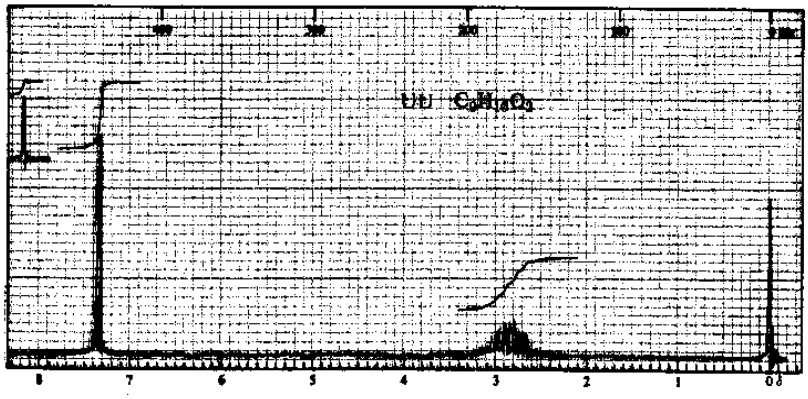
UU Integration: 1, 5, 4

Splitting: 1, 1, multiplet

Formula = $C_9H_{10}O_2$

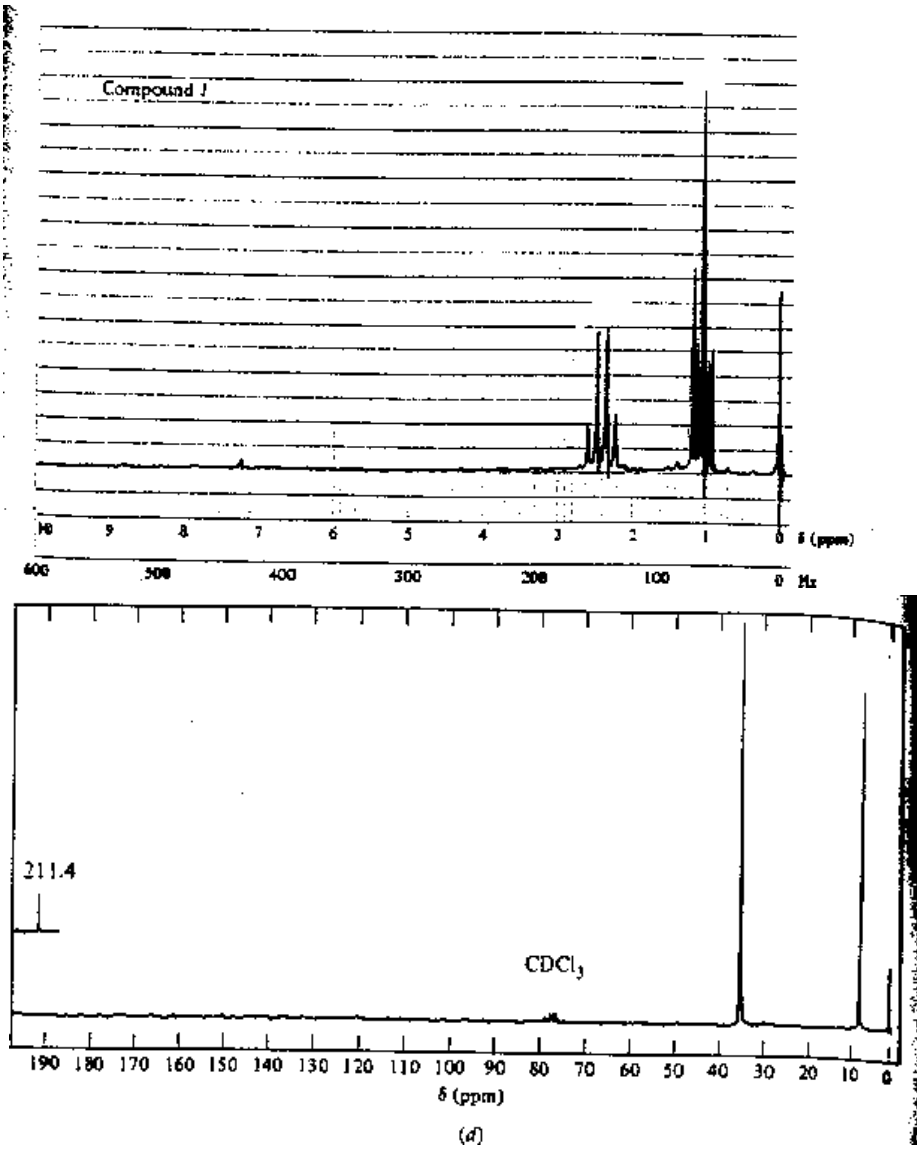




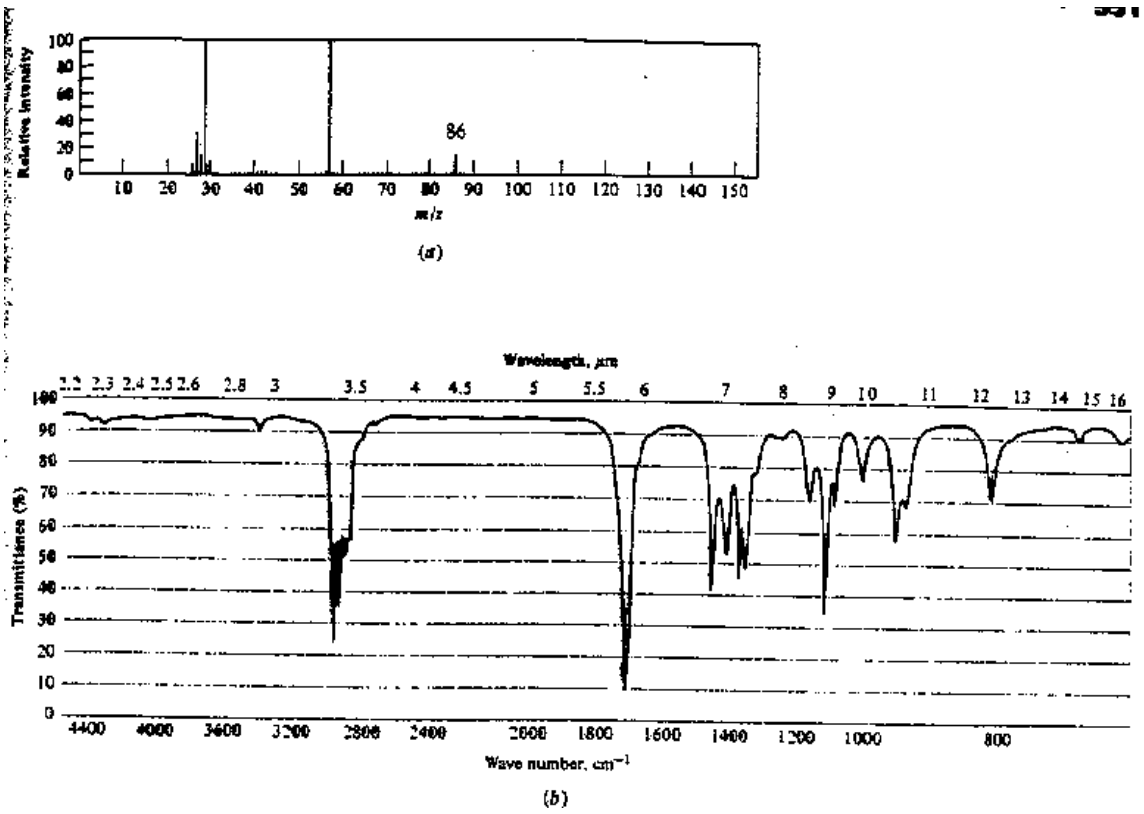


Problem 8

Integration: You guess
Splitting: quartet, triplet
Molecular ion = 86



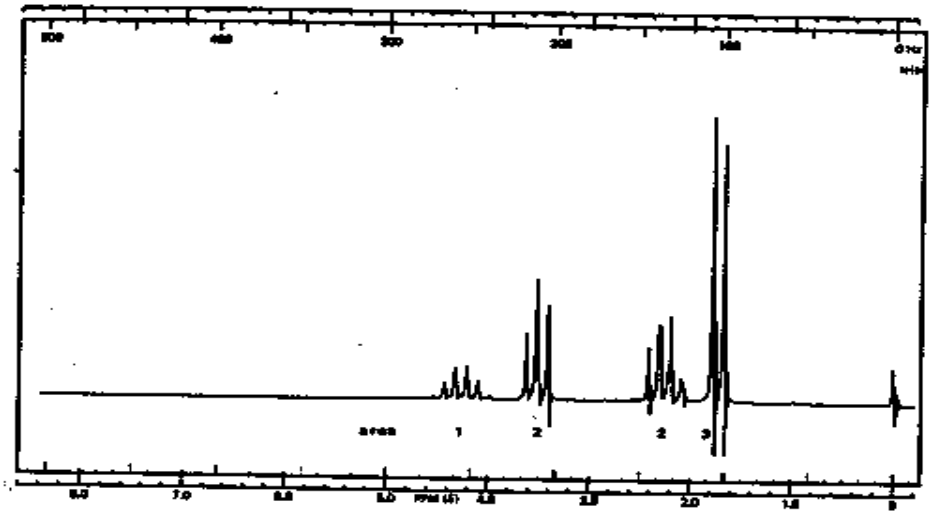
(*d*)


Relative Intensity
100
80
60
40
20
0
86
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
m/z
(a)
Wavelength, μm
2.2 2.3 2.4 2.5 2.6 2.8 3 3.5 4 4.5 5 5.5 6 7 8 9 10 11 12 13 14 15 16
Transmittance (%)
100
90
80
70
60
50
40
30
20
10
0
4400 4000 3600 3200 2800 2400 2000 1800 1600 1400 1200 1000 800
Wave number, cm⁻¹
(b)

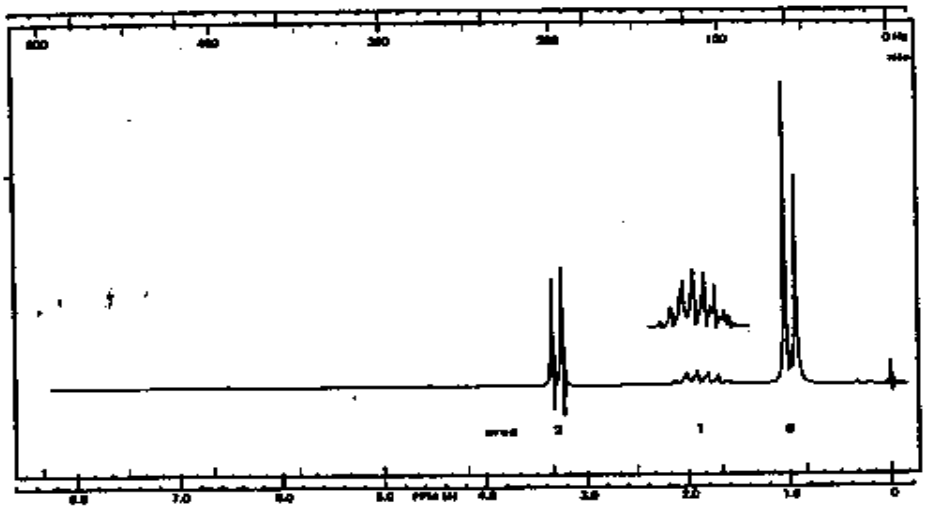
Problem 9

a. Integration values are from low field to high, 1, 2, 2, 3
Splitting is 6, 3, 4, 2
Formula = $C_4H_6Br_2$
b. Integration values are from low field to high, 2, 1, 6
Splitting is 2, 7, 2
Formula = C_4H_9Cl
c. Integration is 2, 4, 3
Splitting is 3, muliplet, 3
Formula = C_4H_9Cl

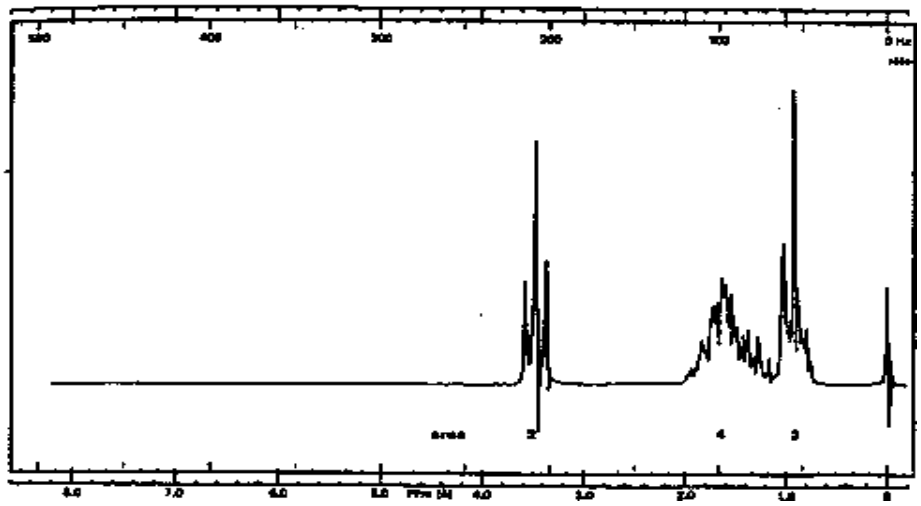
(g) $C_4H_8Br_2$



(h) C_4H_9Cl



(i) C_4H_9Cl

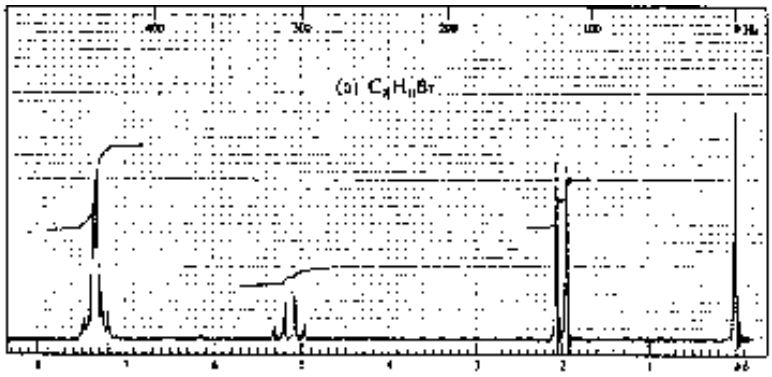


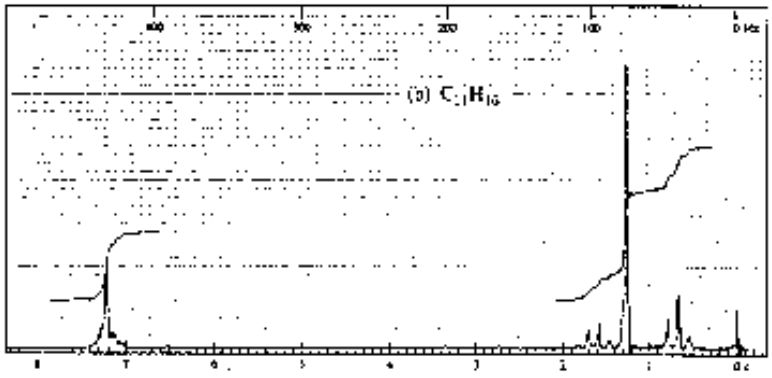
Problem 9 (cont.)

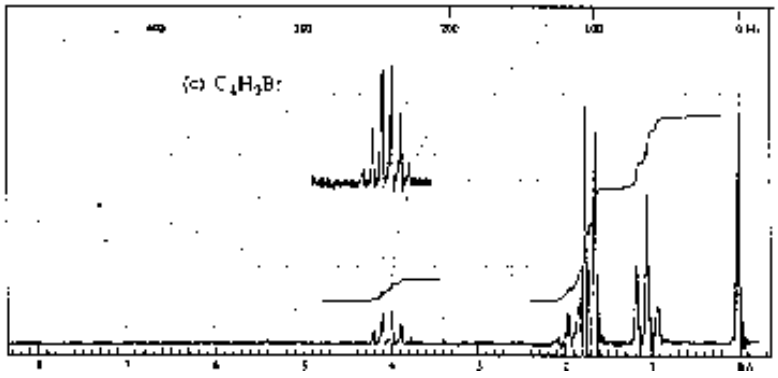
a (d). Integration: 5, 1, 3
Splitting: rough singlet, quartet, doublet
Formula = C_8H_9Br

b (e). Integration: 5, 2, 6, 3
Splitting : singlet, quartet, singlet, triplet
Formula = $C_{11}H_{16}$

c (f). Integration: 1, 5, 3
Splitting: 6, 2 large-many small, 3
Formula = C_4H_9Br



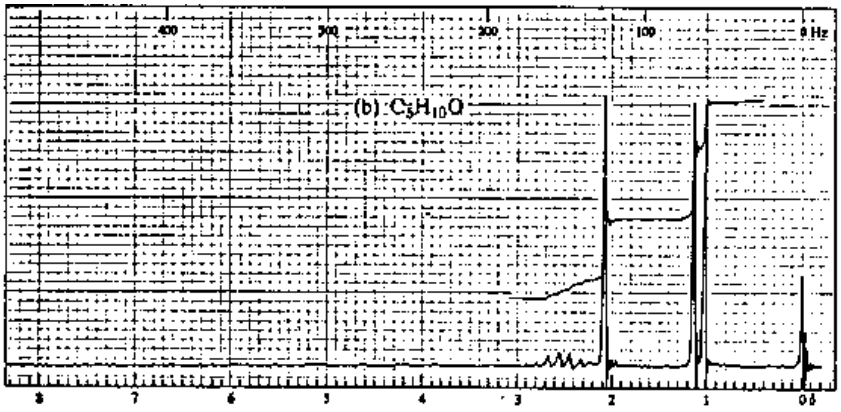


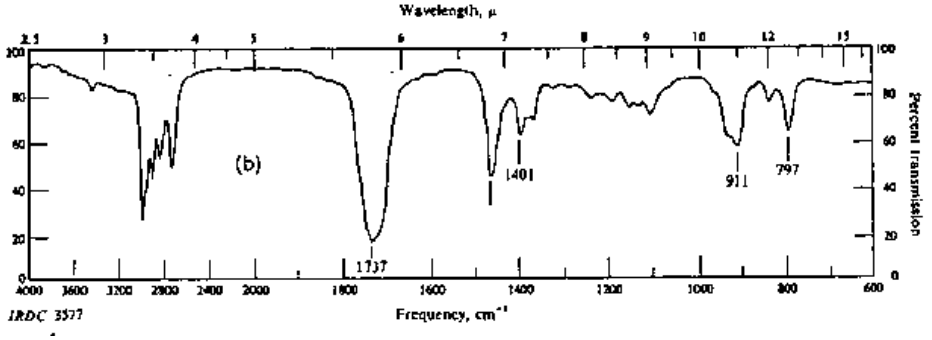


Problem 10

Integration : 1, 3, 6

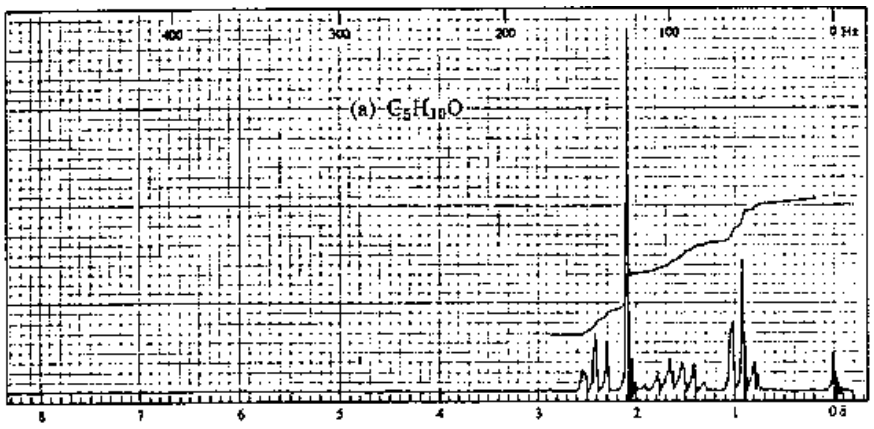
Splitting : multiplet, singlet, doublet
Formula = $C_5H_{10}O$

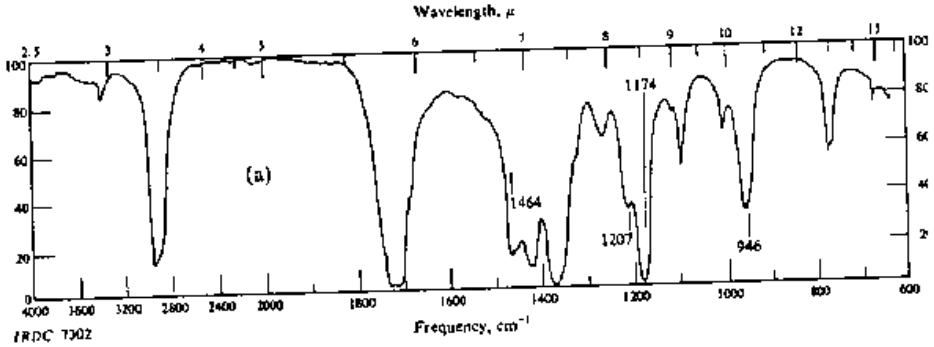




Problem 11

NMR = triplet (2H), singlet(3H), multiplet(2H), triplet(3H)
Formula = C_5H_{10}


(a) $C_5H_{10}O$
400
300
200
100
0 Hz
8
7
6
5
4
3
2
1
0.5


Wavelength, μ
2.5
3
4
5
6
7
8
9
10
12
15
(a)
1464
1174
1207
946
4000
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
Frequency, cm⁻¹
IRDC 7302