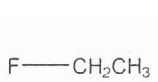
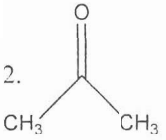
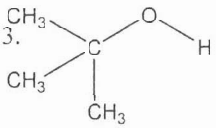
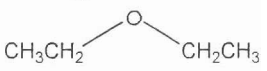
CHEM 235 IN-CLASS #2 NMR ASSIGNMENT (30 pts) Names Key

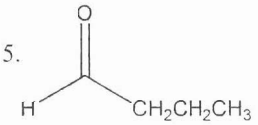
1.Draw the NMR Spectra for the following compounds. Be sure to entail the correct chemical shift, splitting and integration. For chemical shift information you can you can use the table shown below (From page 580 of your text.)

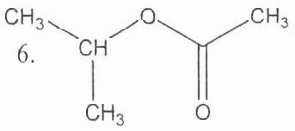
1. 

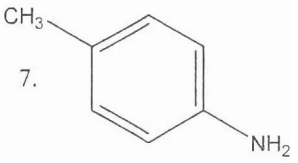
2. 

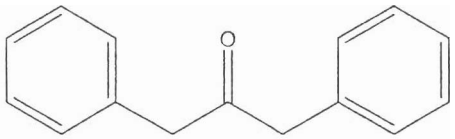
3. 

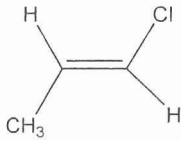
4. 

5. 

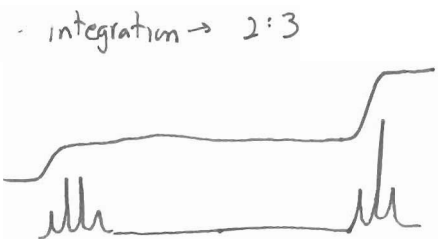
6. 

7. 

8. 

9. 

#1 (example)

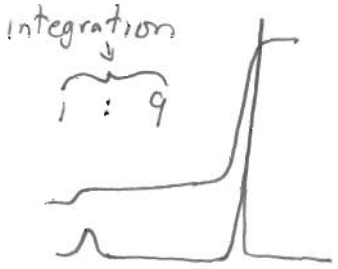


10 9 8 7 6 5 4 3 2 1 0

#2

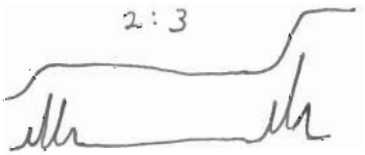
10 9 8 7 6 5 4 3 2 1 0

#3



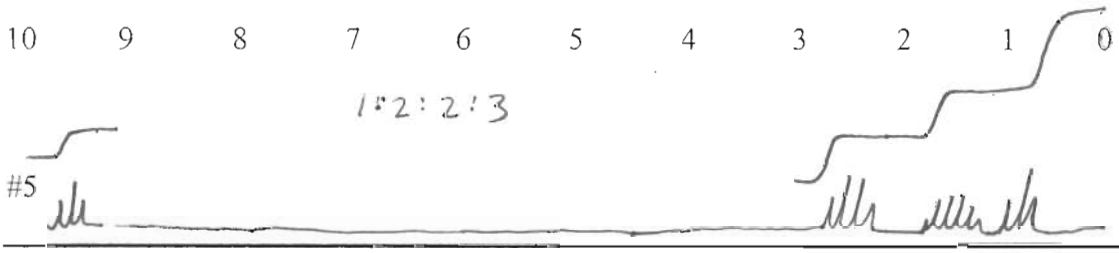
10 9 8 7 6 5 4 3 2 1 0

#4



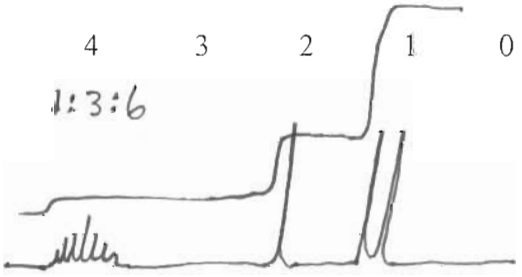
10 9 8 7 6 5 4 3 2 1 0

#5



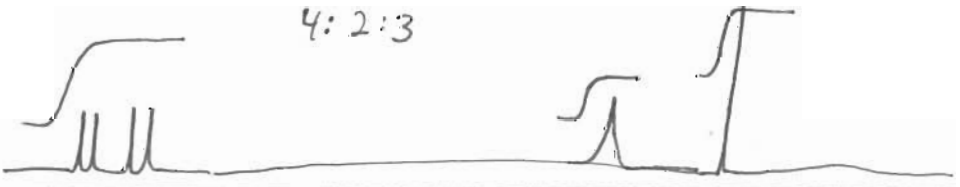
10 9 8 7 6 5 4 3 2 1 0

#6



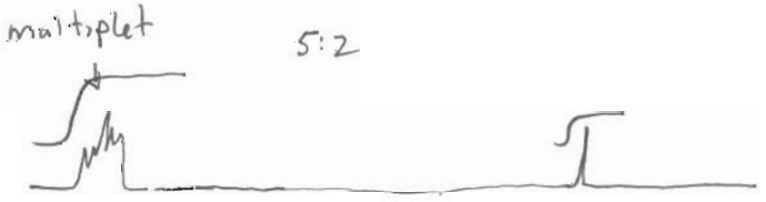
10 9 8 7 6 5 4 3 2 1 0

#7



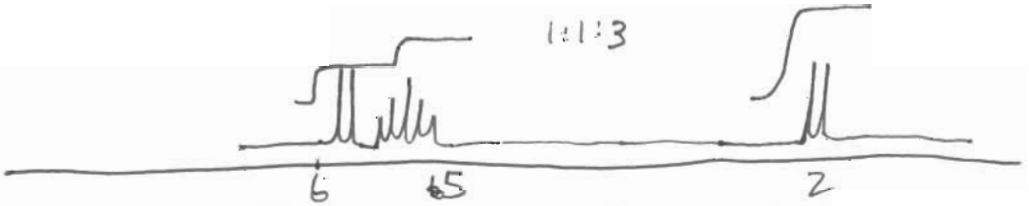
10 9 8 7 6 5 4 3 2 1 0

#8



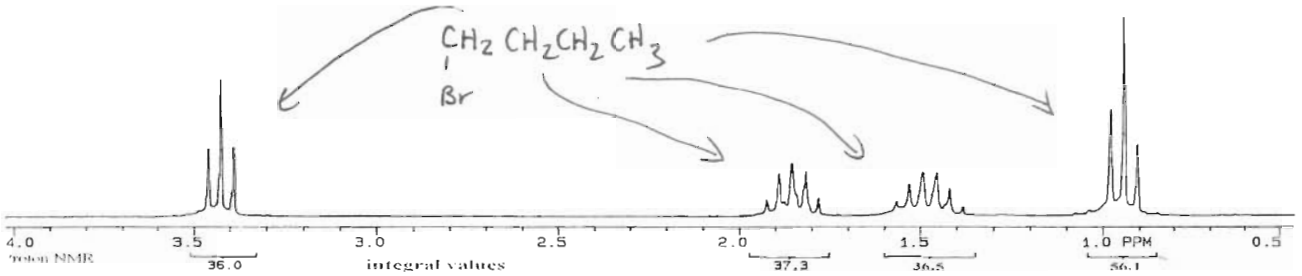
10 9 8 7 6 5 4 3 2 1 0

#9

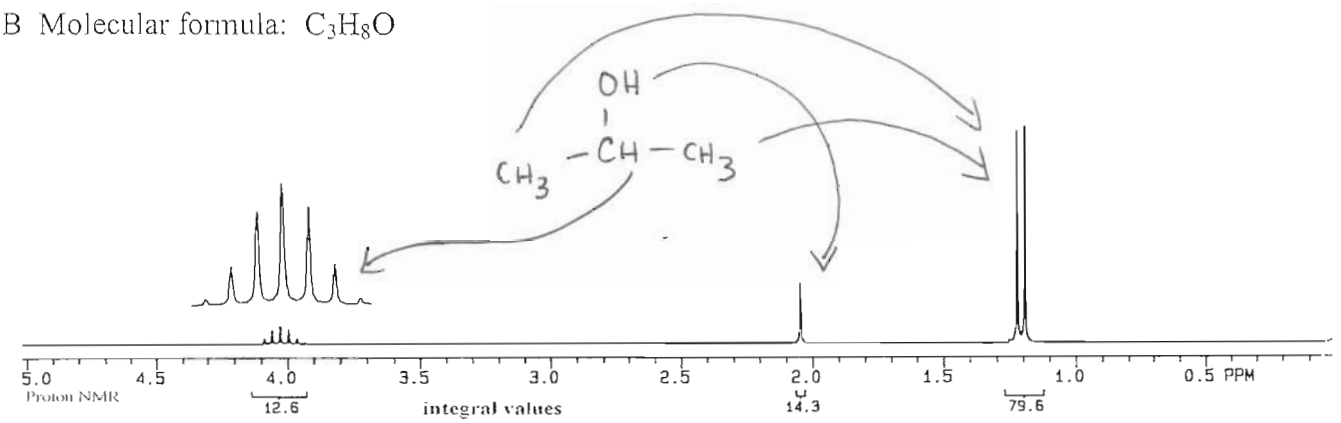


2. For compounds A-E draw in the corresponding structures for the following NMRs. The molecular formula for each unknown compounds is given at the top left hand side of each NMR. The integration values (numbers) listed below each peak

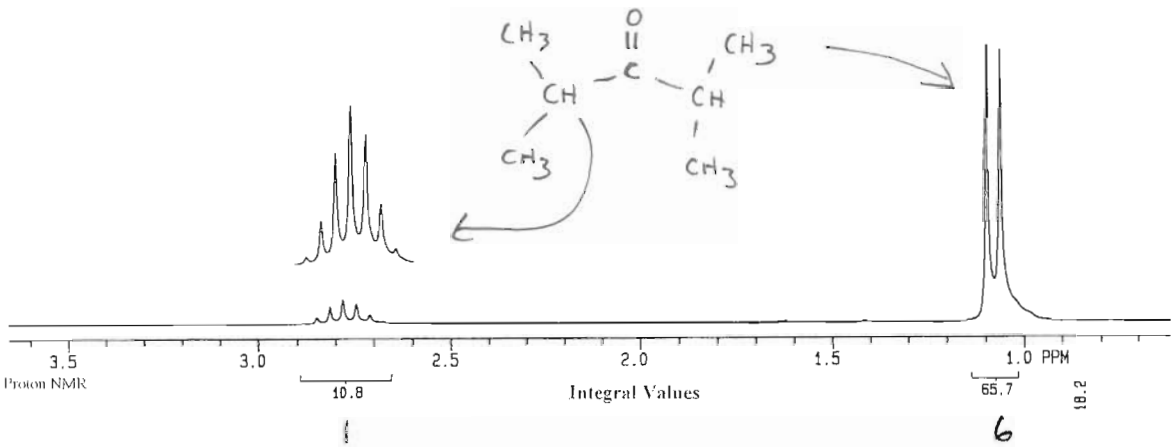
A Molecular formula: C_4H_9Br



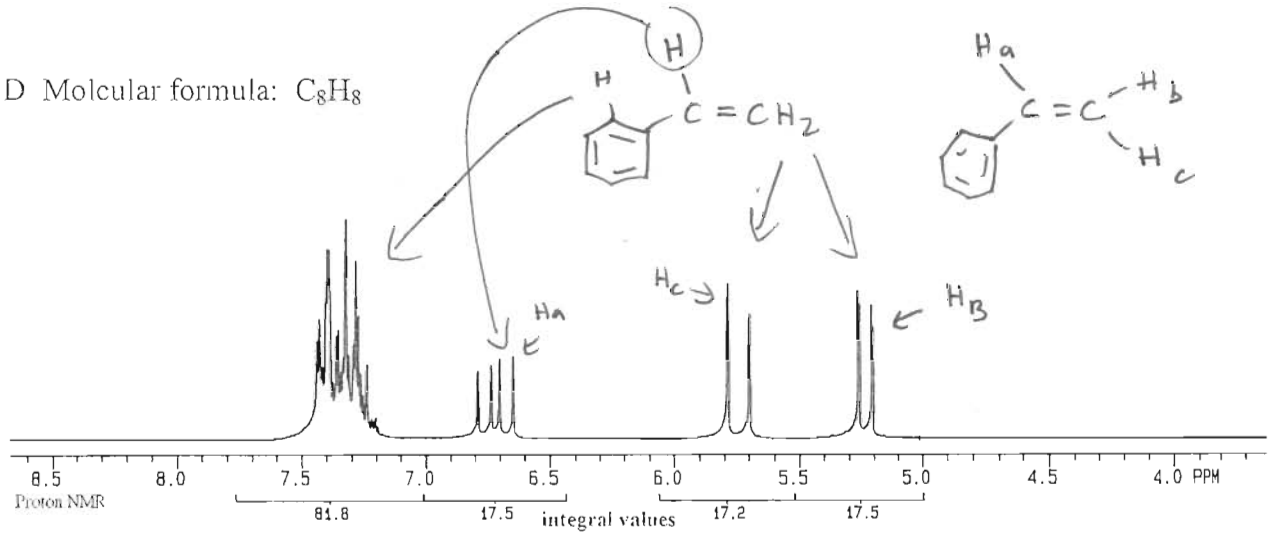
B Molecular formula: C_3H_8O



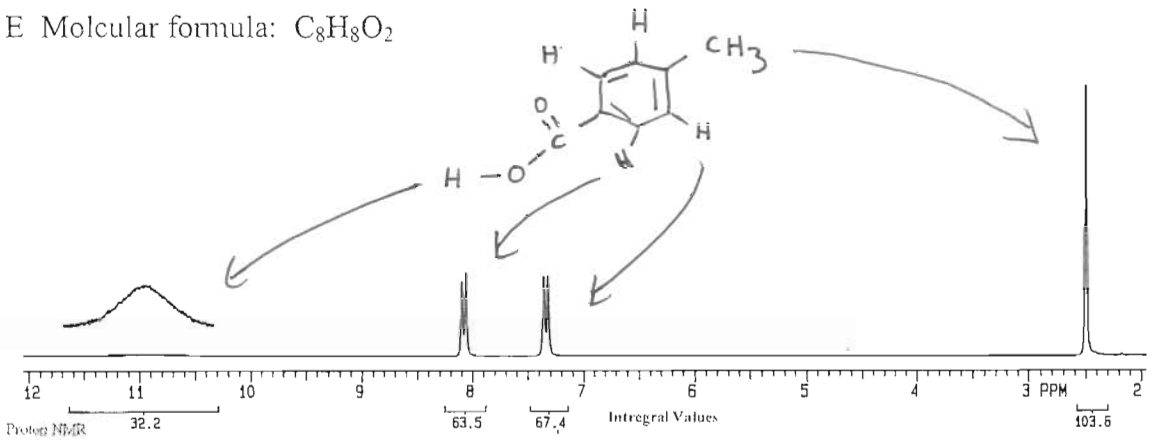
C Molecular formula: $C_7H_{14}O$



D Molcular formula: C_8H_8

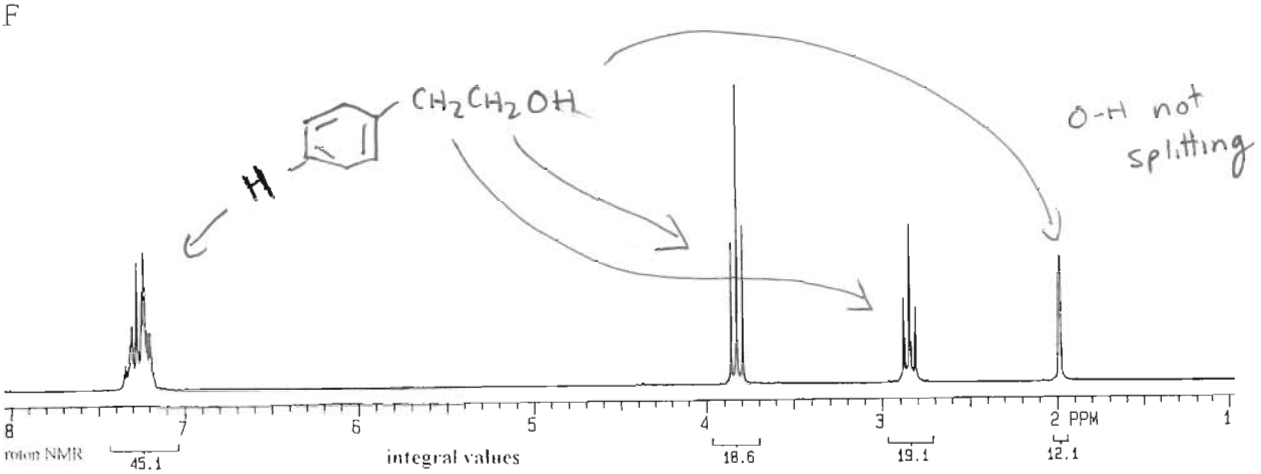


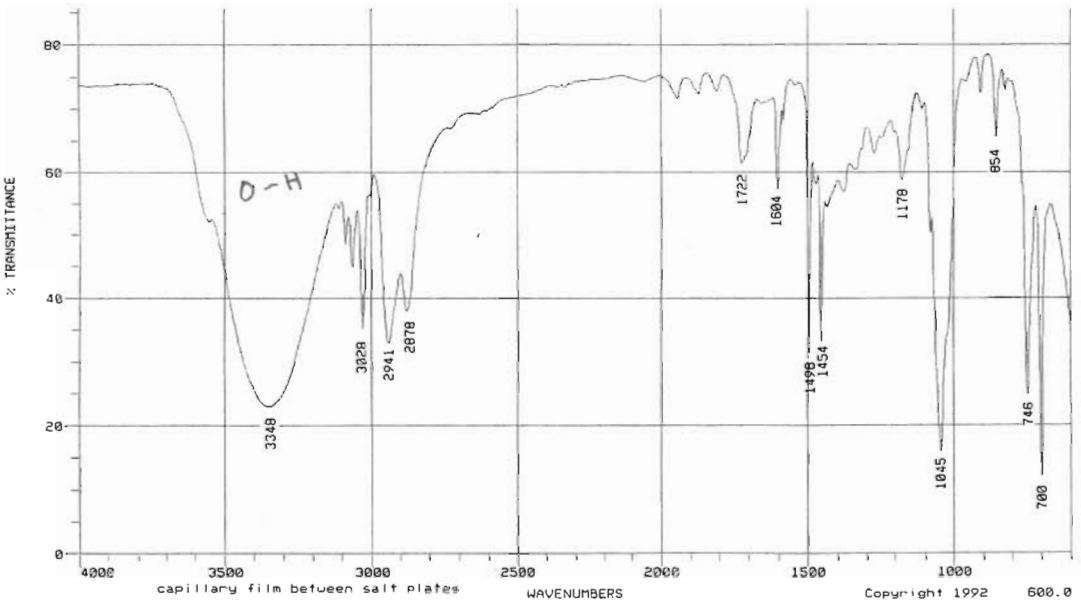
E Molcular formula: $C_8H_8O_2$

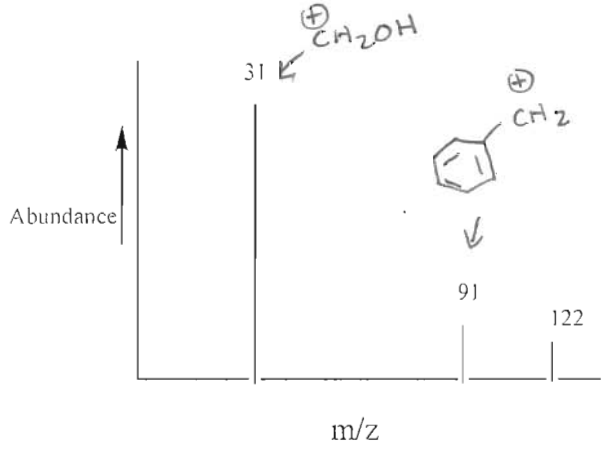


3. Determine the structures of compounds F-I using NMR, IR and Mass spec data.

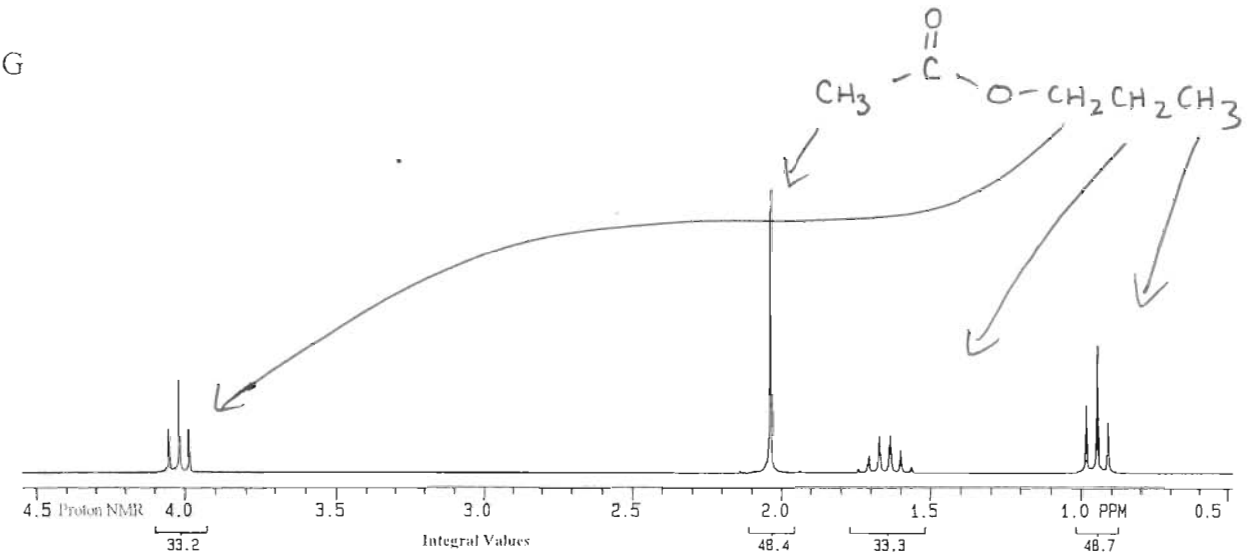
F

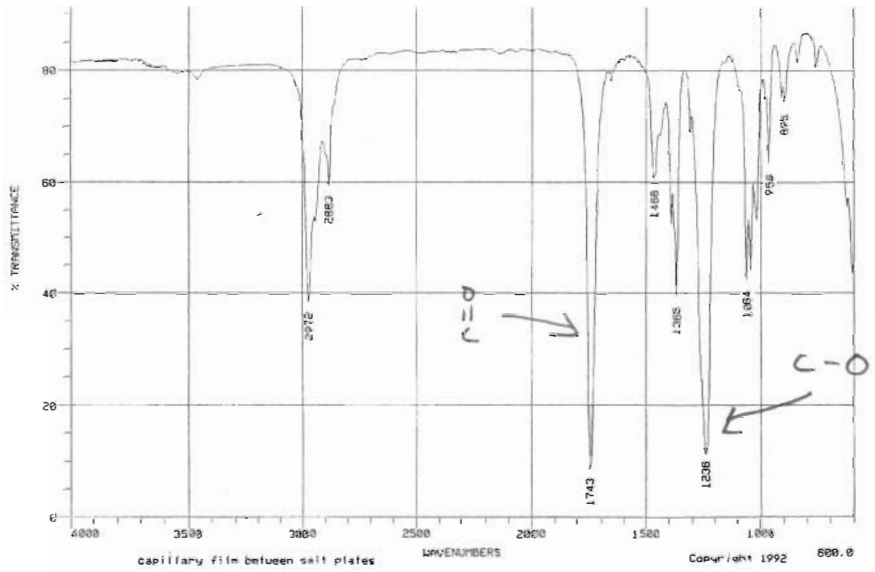


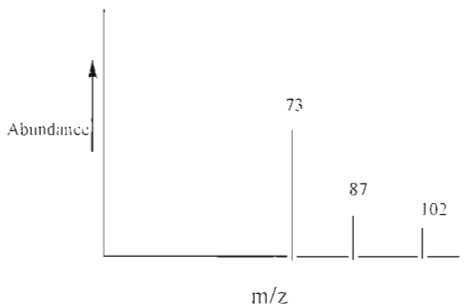




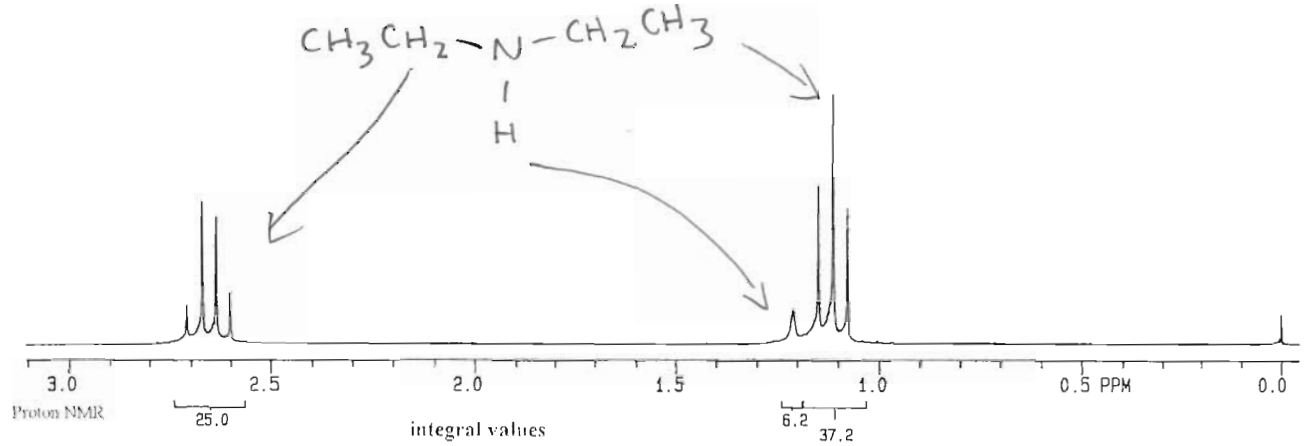
G

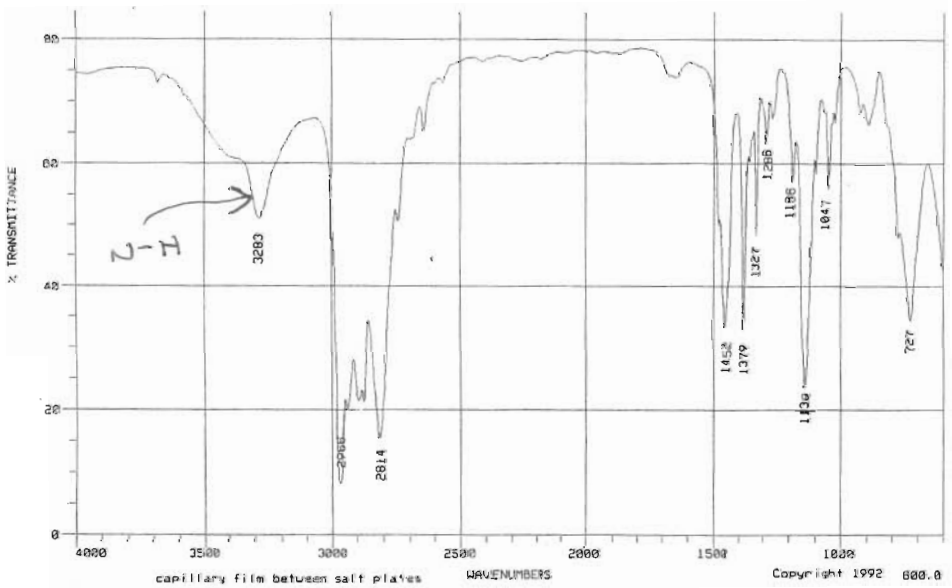

O
C
CH3 - C - O - CH2 CH2 CH3
4.5 Proton NMR
4.0
3.5
3.0
2.5
2.0
1.5
1.0 PPM
0.5
33.2
Integral Values
48.4
33.3
48.7

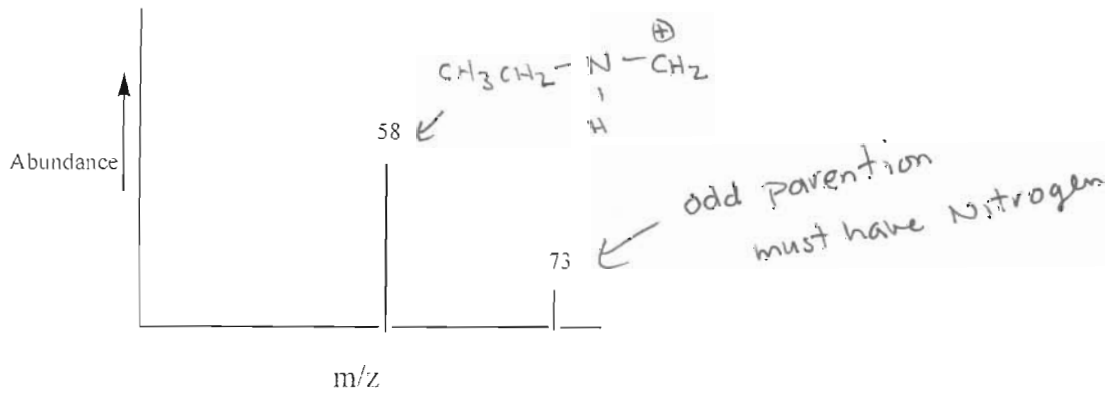

% TRANSMITTANCE
100
80
60
40
20
0
2962
2872
1743
1466
1385
1236
1064
956
895
C=O
C-O
4000
3500
3000
2500
2000
1500
1000
500.0
WAVENUMBERS
capillary film between salt plates
Copyright 1992


Abundance
73
87
102
m/z

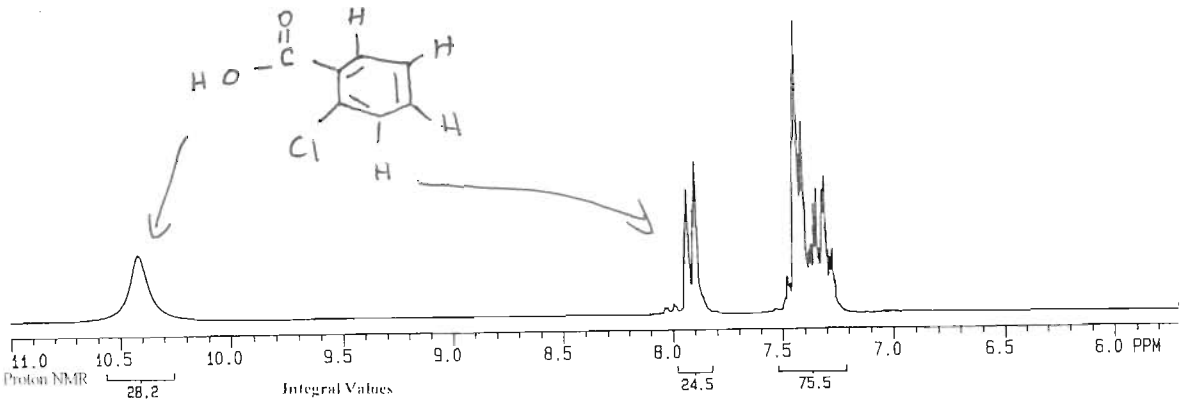
H

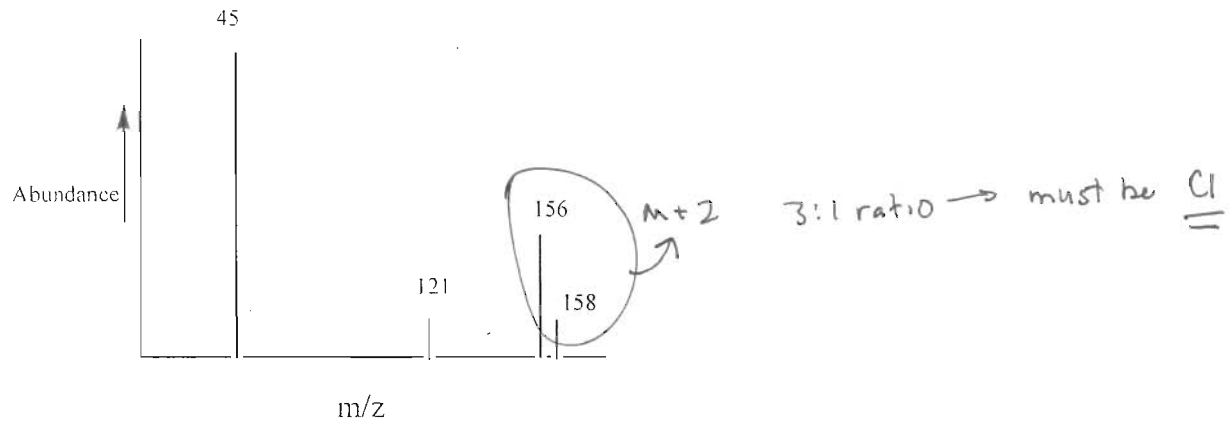

CH3CH2-N-CH2CH3
H
3.0
2.5
2.0
1.5
1.0
0.5 PPM
0.0
Proton NMR
25.0
integral values
6.2
37.2


% TRANSMITTANCE
N-H
3283
2956
2814
1458
1379
1327
1288
1186
1130
1047
727
4000
3500
3000
2500
2000
1500
1000
capillary film between salt plates
WAVENUMBERS
Copyright 1992
800.0


CH3CH2-N-CH2
H
58
Abundance
odd parention
must have Nitrogen
73
m/z

I


11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0 PPM
Proton NMR
28.2
Integral Values
24.5
75.5


45
Abundance
156
121
158
m+2
3:1 ratio → must be Cl
m/z