Identify each peak and comment on the utility of this effect in the interpretation of NMR spectra. Repeat the experiment using 2-propanol or 2-methyl-2-propanol.

C. CARBON-13 SPECTRUM OF ETHYLBENZENE

This experiment is designed to illustrate the effect of proton decoupling on a carbon-13 spectrum. Decoupled spectra are less complex than "nondecoupled" spectra because the splitting of the carbon signal by hydrogen is absent.

1. Determine the ^{13}C spectrum of the ethylbenzene sample used in Experiment A using the following conditions:
   a. Normal, decoupled power applied.
   b. Decoupling power turned off.

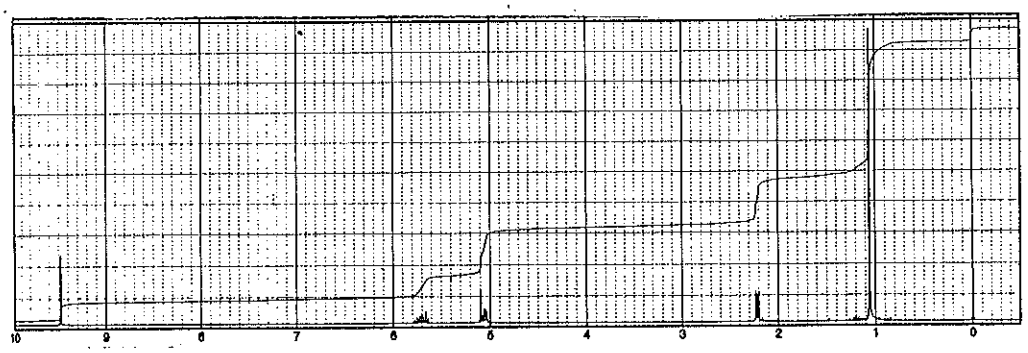
Overlay the two spectra, line up the TMS peaks, and record the identity and splitting patterns for each peak of the sample.

D. ACQUIRE THE SPECTRA OF AN UNKNOWN COMPOUND SUPPLIED BY YOUR INSTRUCTOR, AND DETERMINE THE STRUCTURE

PROBLEM 13.1

$C_7H_{12}O$

^{13}C NMR	^{1}H NMR
206.7, d	1.08, s, 6H
133.1, d	2.21, d, J = 7.2 Hz, 2H
118.4, t	5.08, d, J = 11.8 Hz, 1H
45.7, s	5.11, d, J = 15.5 Hz, 1H
41.5, t	5.75, ddt, J = 11.8, 15.5, 7.2 Hz, 1H
21.2, q (2)	9.49, s, 1H

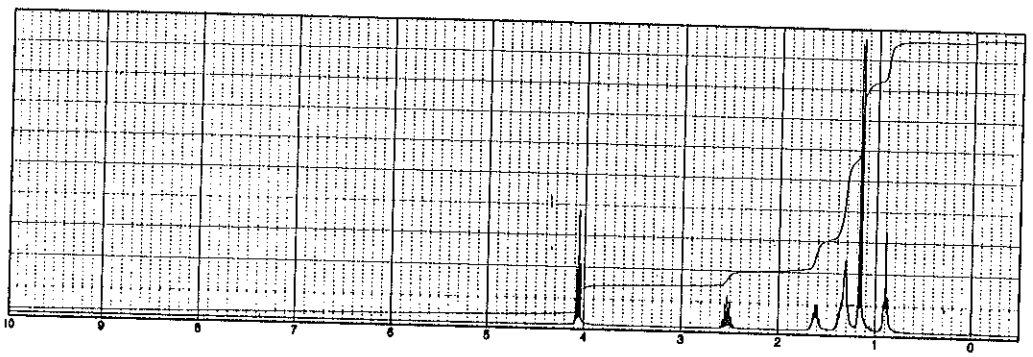


PROBLEM 13.2

$C_{10}H_{20}O_2$

^{13}C NMR
177.0, s
64.4, t
34.1, d
31.6, t
28.8, t
25.7, t
22.6, t
19.1, q (2)
14.0, q

^{1}H NMR
0.89, t, J = 7.3 Hz, 3H
1.26, d, J = 6.5 Hz, 6H
1.4, m, 6H
1.64, m, 2H
2.52, m, 1H
4.05, t, J = 7.1 Hz, 2H

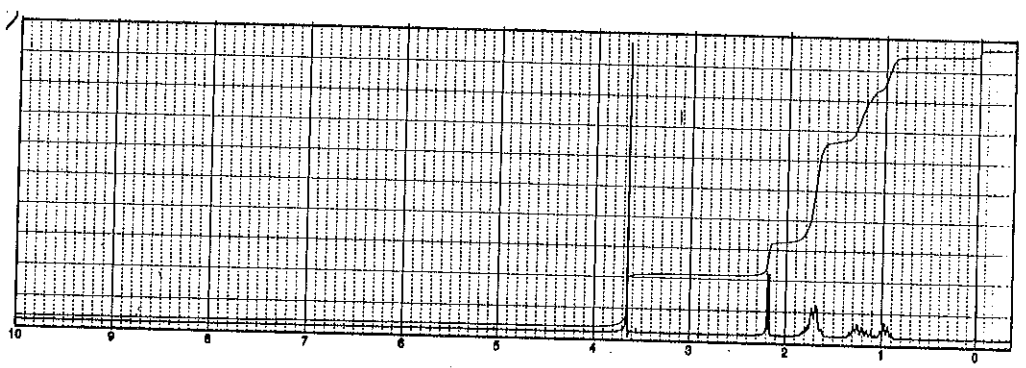


PROBLEM 13.3

$C_9H_{16}O_2$

^{13}C NMR
173.6, s
51.3, q
42.0, t
34.9, d
33.1, t (2)
26.2, t (2)
26.1, t

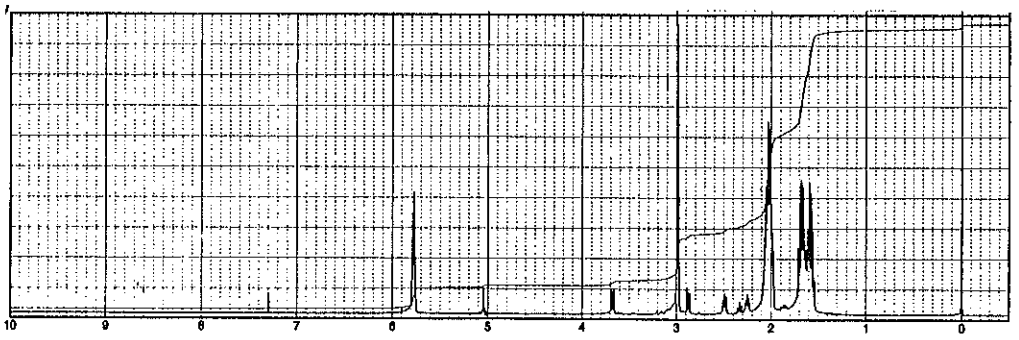
^{1}H NMR
3.67, s, 3H
2.19, d, J = 6.4 Hz, 2H
1.70, m, 6H
0.9–1.3, m, 5H



PROBLEM 13.4

$C_8H_{11}N$

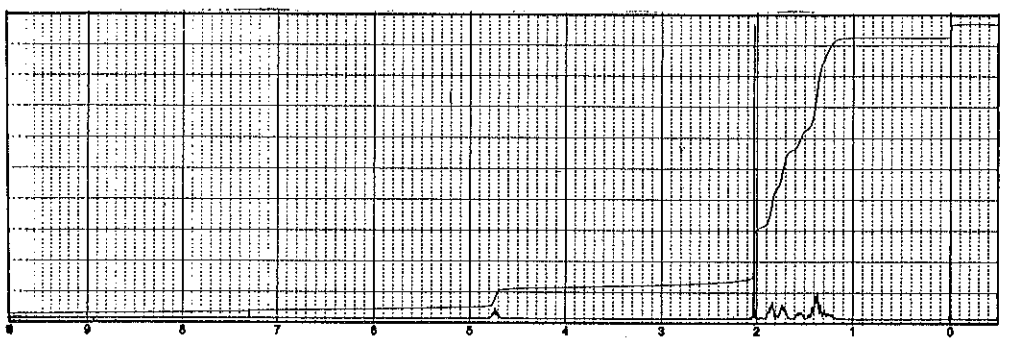
^{13}C NMR	^{1}H NMR
127.1, s	5.79, t, J = 6.2 Hz, 1H
126.3, d	2.97, s, 2H
117.7, s	2.02, m, 4H
28.0, t	1.70, m, 4H
25.8, t	
25.1, t	
22.5, t	
21.8, t	



PROBLEM 13.5

$C_8H_{14}O_2$

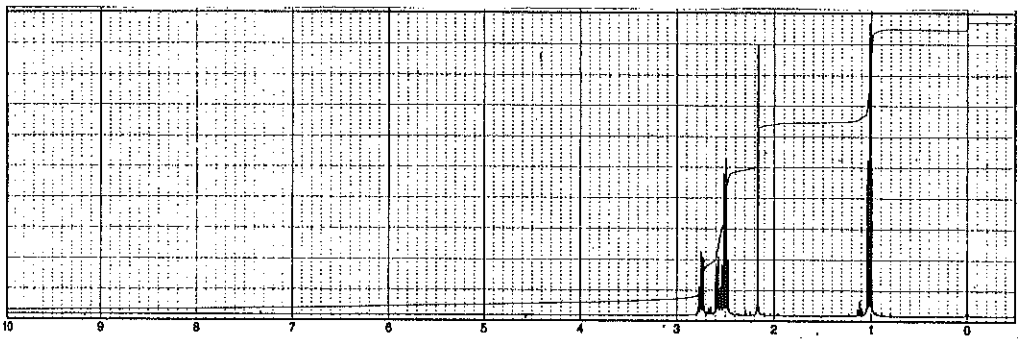
^{13}C NMR	^{1}H NMR
170.5, s	4.75, m, 1H
72.6, d	2.03, s, 3H
31.7, t (2)	1.2–1.7, m, 10H
25.4, t	
23.8, t (2)	
21.4, q	



PROBLEM 13.6

$C_8H_{17}NO$

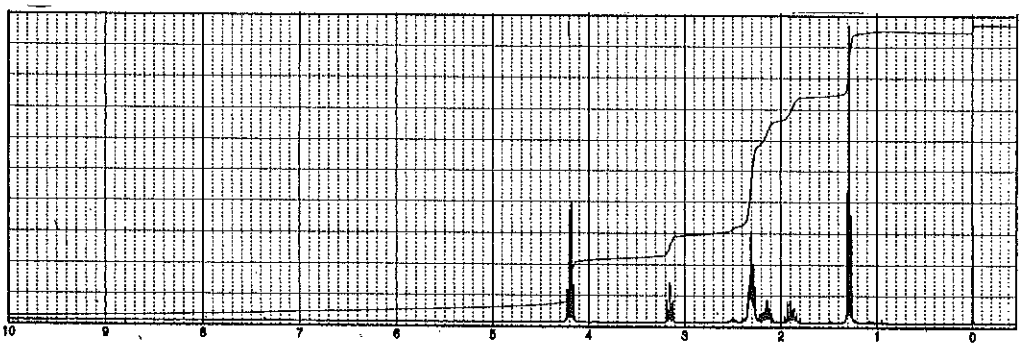
^{13}C NMR	^{1}H NMR
208.2, s	1.02, t, J = 7.1, 6H
47.5, t	2.16, s, 3H
46.9, t	2.52, t, J = 7.1 Hz, 4H
41.6, t (2)	2.61, t, J = 7.6 Hz, 2H
30.2, q	2.75, t, J = 7.6 Hz, 2H
11.8, q (2)	



PROBLEM 13.7

$C_8H_{12}O_3$

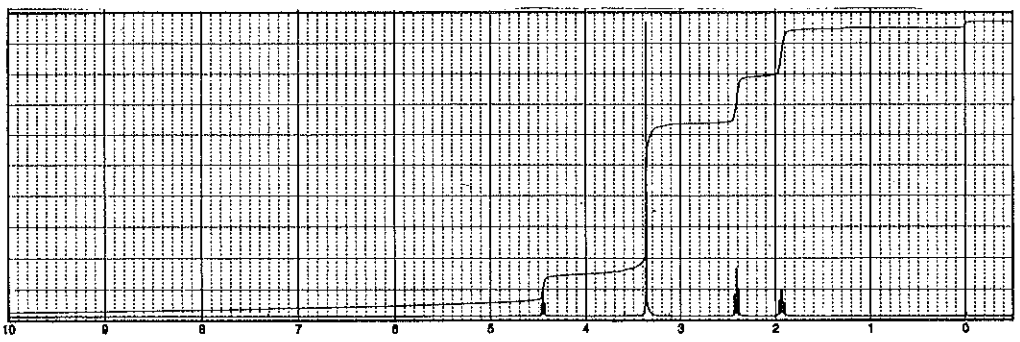
^{13}C NMR	^{1}H NMR
212.3, s	1.28, t, J = 7.2 Hz, 3H
169.4, s	1.9–2.1, m, 2H
61.3, t	2.3, m, 4H
54.8, d	3.15, t, J = 8.4 Hz, 1H
38.0, t	2.39, q, J = 7.2 Hz, 2H
27.4, t	
21.0, t	
14.2, q	



PROBLEM 13.8

$C_6H_{11}NO_2$

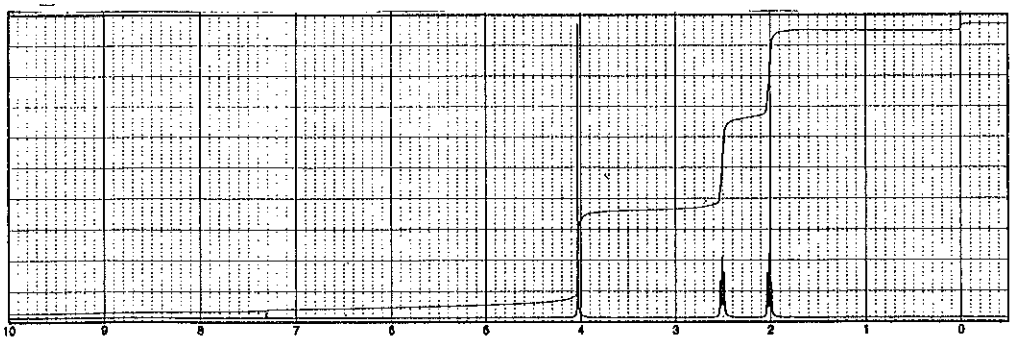
^{13}C NMR	^{1}H NMR
119.4, s	4.46, t, J = 6.2 Hz, 1H
102.7, d	3.36, s, 6H
53.8, q (2)	2.41, t, J = 7.4 Hz, 2H
28.5, t	1.92, dt, J = 6.2, 7.4 Hz, 2H
12.4, t	



PROBLEM 13.9

$C_8H_{12}O_3$

^{13}C NMR	^{1}H NMR
210.1, s	4.04, s, 4H
107.1, s	2.50, t, J = 6.6 Hz, 4H
64.6, t (2)	2.02, t, J = 6.6 Hz, 4H
38.2, t (2)	
33.9, t (2)	



PROBLEM 13.10

$C_9H_{17}NO$

^{13}C NMR	^{1}H NMR
171.1, s	0.96, d, J = 7.8 Hz, 6H
46.8, t (2)	1.9, m, 4H
43.7, t	2.18, d, J = 6.8 Hz, 2H
26.1, t (2)	2.40, m, 1H
25.5, d	3.44, m, 4H
22.7, q (2)	

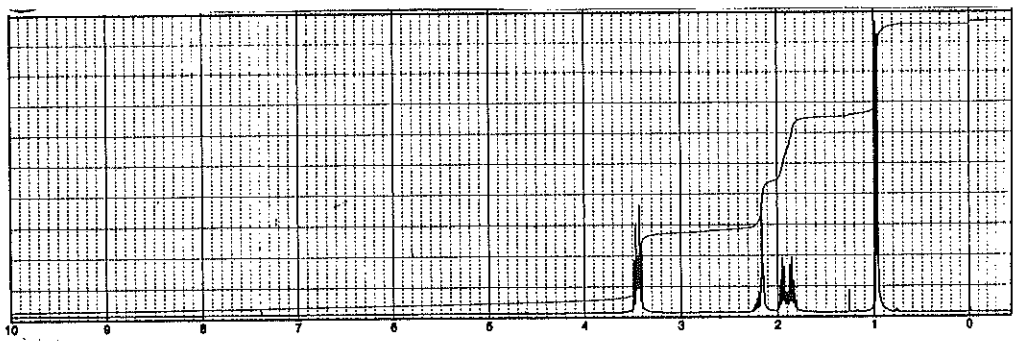


Table 13.1 Chemical Shifts of Protons on a Carbon Atom Adjacent (α Position) to a Functional Group in Aliphatic Compounds (M—Y)

| M = methyl
8 M = methylene
M = methine