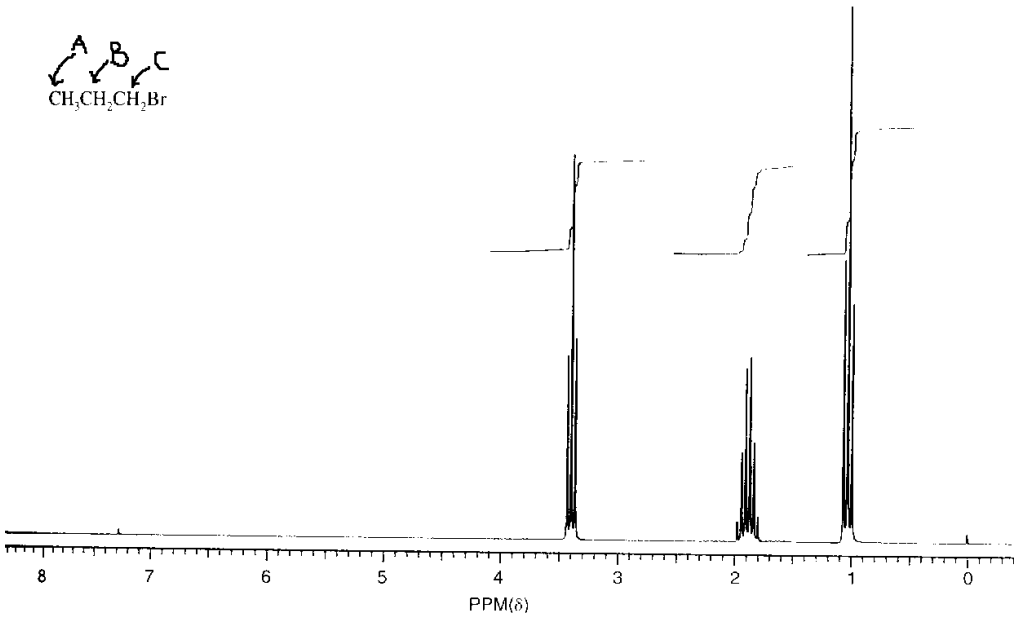
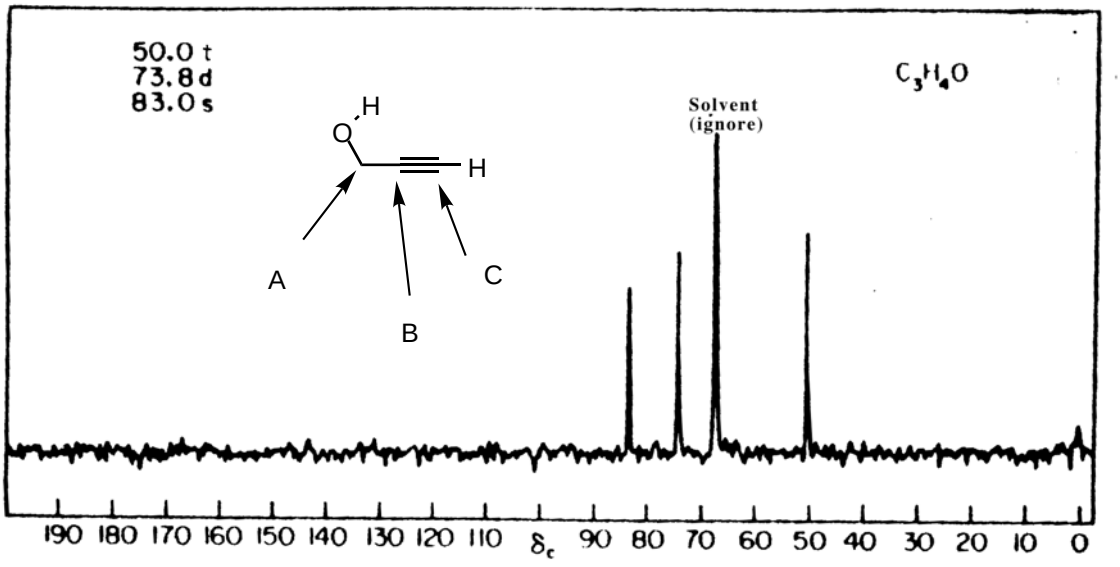
CHEM333 Problem Set 1.
C-13 and H-1 NMR

1a. Assign the proton NMR resonances of 1-bromopropane. (Draw the letter above the corresponding proton NMR resonance) Explain your reasoning.

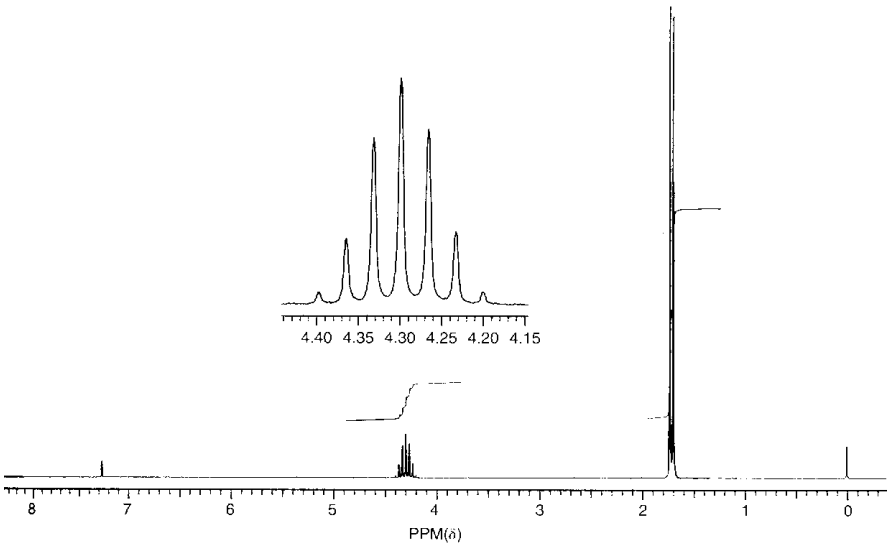


1b. Assign ^{13}C-NMR spectrum of propyne-3-ol. Explain your reasoning.

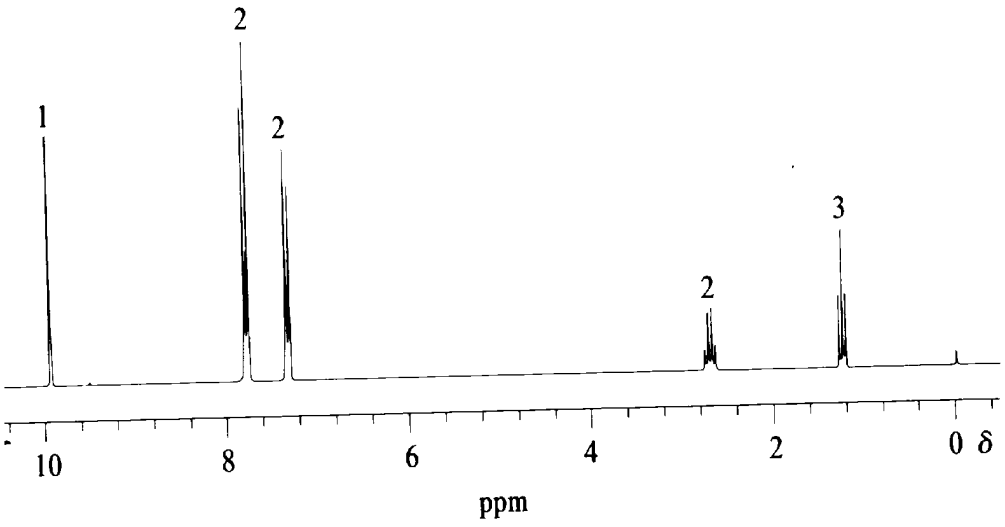


2. Proton NMR

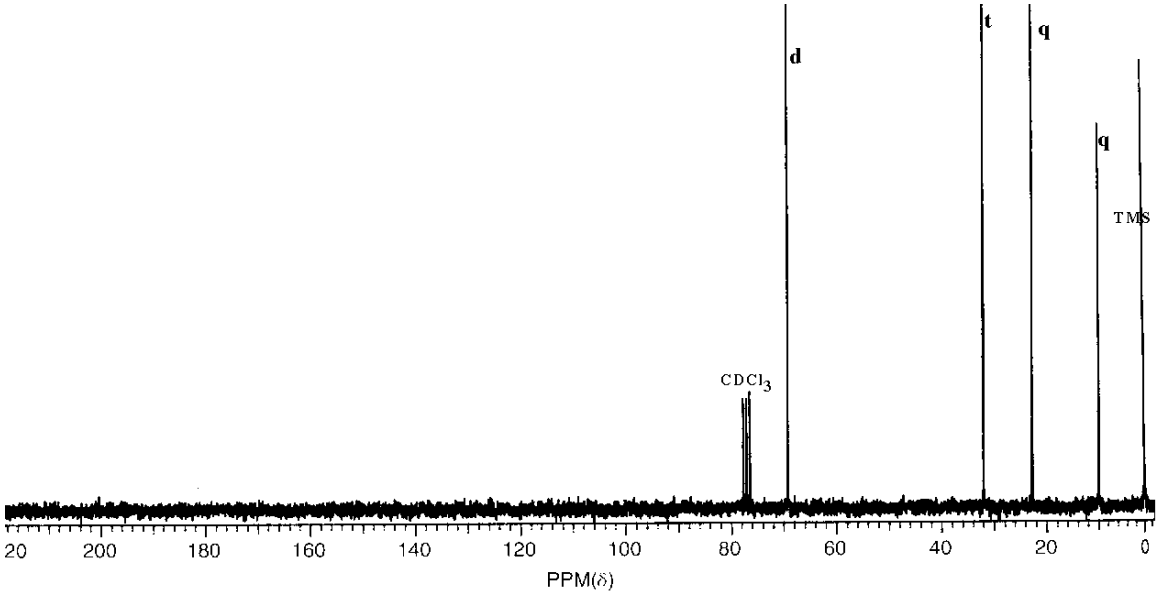
2a. Propose a structure for the compound with molecular formula C_3H_7Br whose proton NMR is shown below. (Hint: The two resonances have an area ratio of 1:6.)



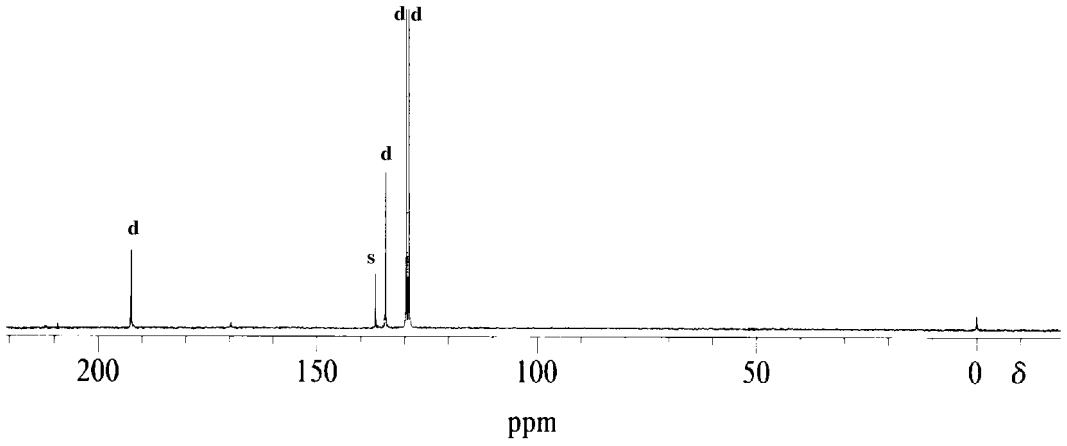
2b. Propose a structure for the compound with molecular formula $C_9H_{10}O$. Explain your reasoning.



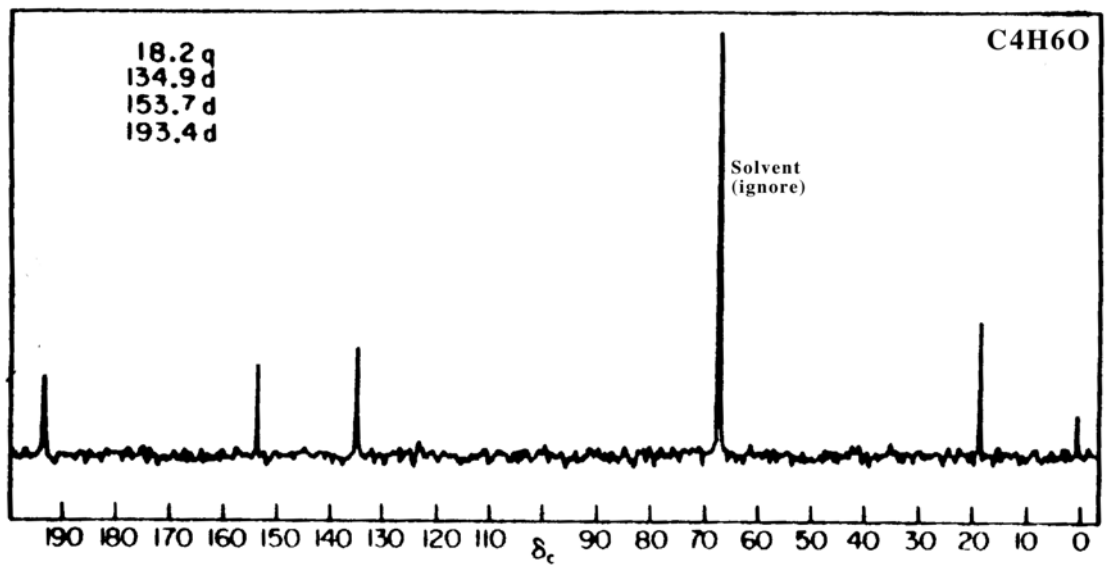
3a. Propose a structure for the compound of molecular formula $C_4H_{10}O$ whose ^{13}C-NMR is shown. Explain your reasoning.



3b. Propose a structure for the compound with molecular formula C_7H_6O whose ^{13}C-NMR spectrum is shown. Explain your reasoning.



3d. Propose a structure for the compound with molecular formula C_4H_6O whose ^{13}C-NMR spectrum is shown. Explain your reasoning



4. C_9H_{16} (25 points)

$\underline{C}^{13}$ NMR
159.7, s
102.0, t
31.2, s
29.7, d
12.9, q (3 carbons)
7.2, t (2 carbons)

5. $C_9H_{18}O$ (25 points)

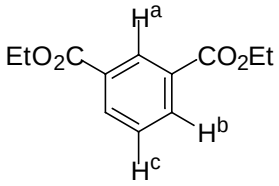
$\underline{C}^{13}$ NMR
210.6, s
52.4, t (2 carbons)
24.5, d (2 carbons)
22.6, q (4 carbons)

6. $C_6H_{11}BrO_2$ (25 points)

$\underline{C}^{13}$ NMR
173.4, s

51.5, q
33.1, t
32.9, t
32.0, t
23.5, t

6. 'Draw' the ^{1}H NMR spectrum of the compound **2**. The chemical shift information is given, but it is your task to illustrate the coupling patterns.



H^a: δ = 8.7 ppm
H^b: δ = 8.2 ppm
H^c: δ = 7.5 ppm

2

7. Determine the structure:
: C_6H_8O

C^{13} NMR
200, s
150, d
130, d
38, t
25, t
22, t

8. Determine the structure.
$C_9H_{10}O$

C^{13} NMR

135, s
133, s
129, d
126.3, d
125.9, d
124. d
68, t
65, t
28, t