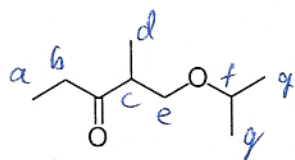1. Predict the ^{1}H NMR spectrum. Include approximate chemical shifts (1's, 2's, etc.), the integration, and the splitting (can use "s" for singlet; "d" for doublet; "t" for triplet; "q" for quartet, and "m" for multiplet, anything more complex than a quartet). Note: for signals that are symmetry equivalent, do not list them twice.
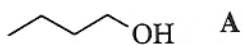
a   1's 3H   t   e   3's 2H d

b   2's 2H   q   f   3's 1H m

c   2's 1H   m   g   1's 6H d

d   1's 3H   d

2. Predict the ^{13}C NMR spectrum. Include the approximate chemical shifts (220-160, 160-100, 100-50, or 50-0) and the splitting (q, t, d, s).
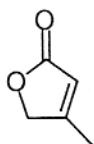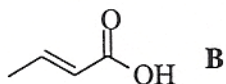
220 -160 S   100-50 t

160-100 d   50-0 q

160-100 S

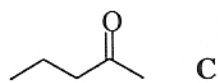3. Match the following structures with the listed feature IR signals.

OH   A   1710   C

OH   B   3300-3400   A

C   C   1680, 3300-2500   B

Solve the Structures for the Following. If you get a structure perfect, you will get full credit. If you do not get a structure perfect, you may still get some partial credit. Thus, it is in your interest to show some of your work, make a structure, or tell me what you know for sure.

4. $C_5H_{12}O$ IR: Nothing Interesting   ⇒ ether

$C_5H_{12}O$

3H

2H

3H

3H

1H

4   3   2   1

$$CH_3$$
$$|$$
$$CH_3O\ CH$$
$$|$$
$$CH_2$$
$$|$$
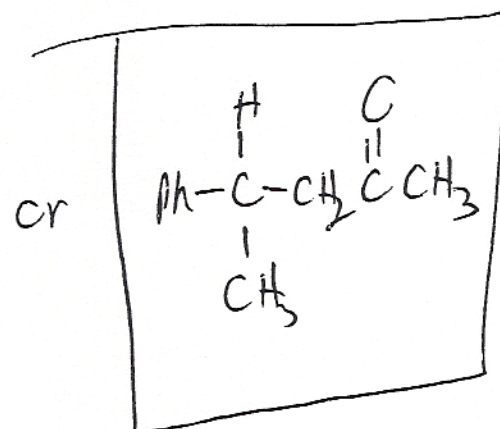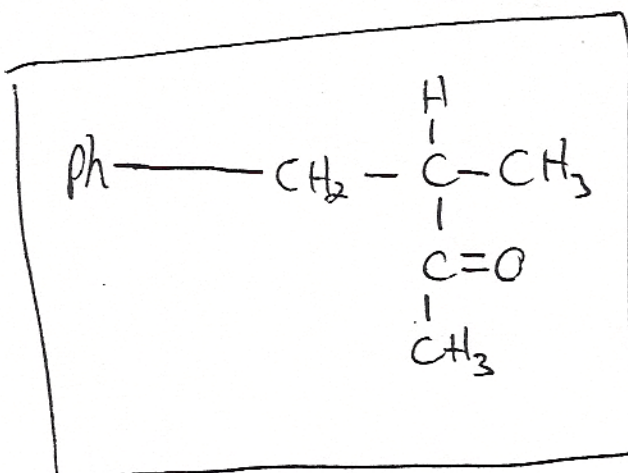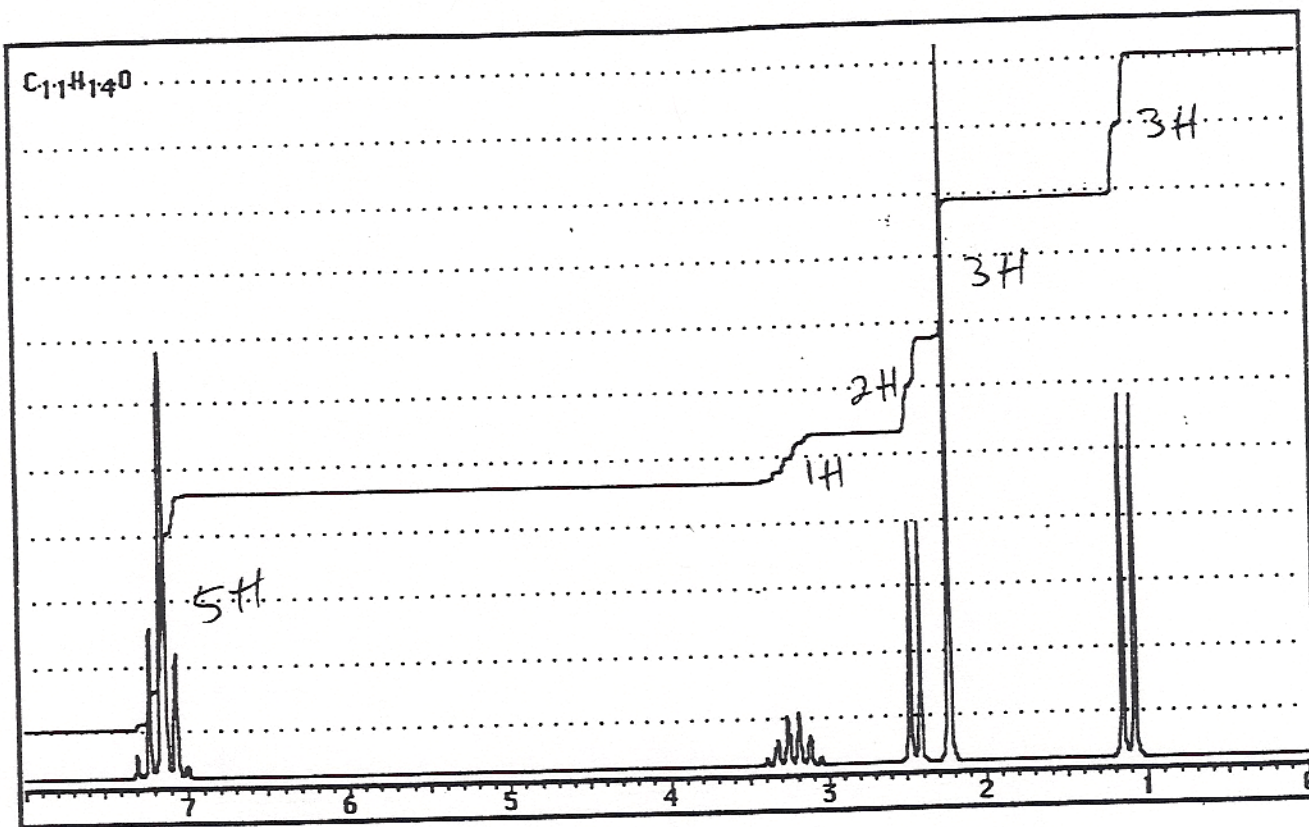$$CH_3$$
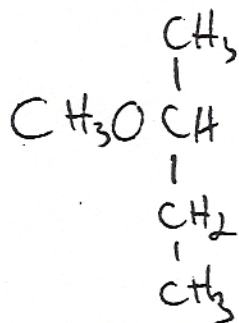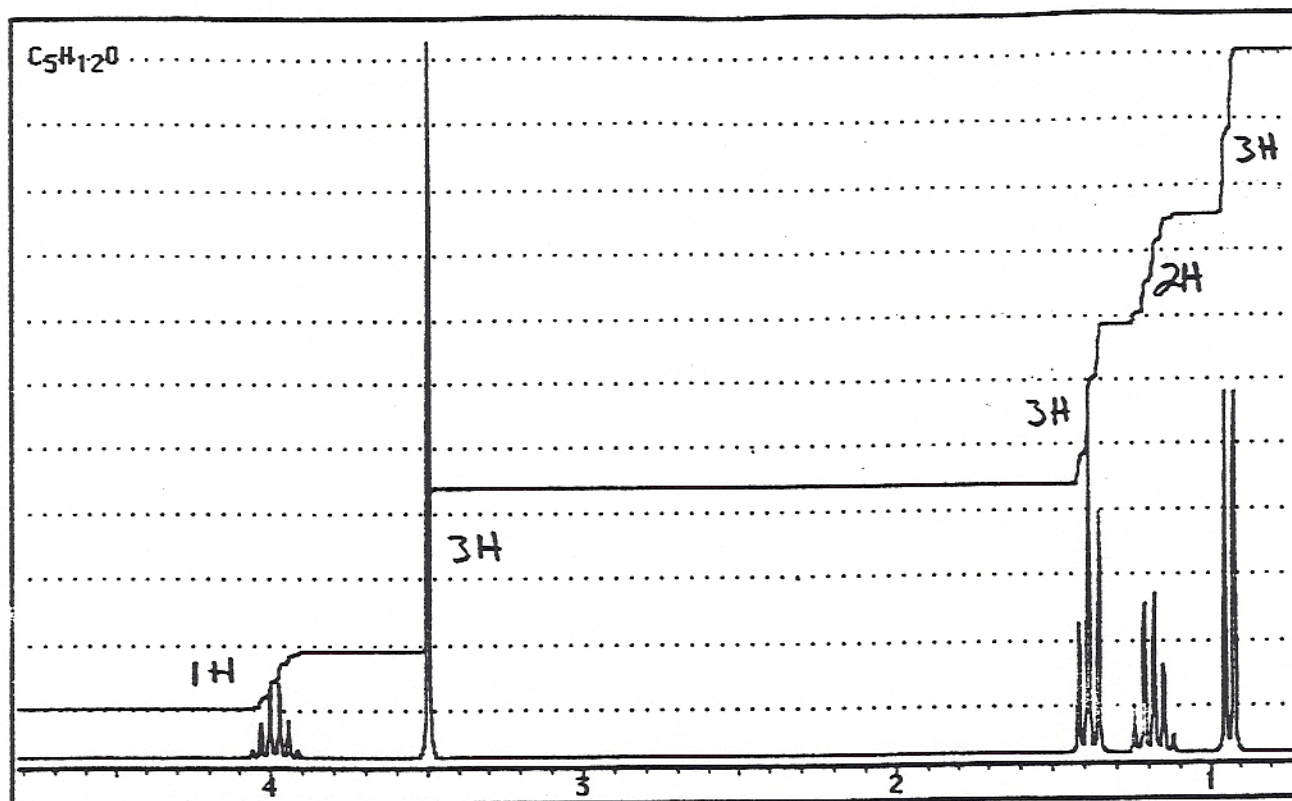
5. $C_{11}H_{14}O$ IR: 1710   C=O, not conjugated   error (+)

^{13}C NMR: 202 (s), 152 (s), 134 (d), 127 (d), 122 (d), 42 (d), 35 (q), 20 (q)

EU= 5

$C_{11}H_{14}O$

3H

3H

2H

1H

5H

Ph————CH_2 — $\overset{\overset{H}{|}}{\underset{\underset{\underset{CH_3}{|}}{\underset{C=O}{|}}}{C}}$—$CH_3$

or

Ph—$\overset{\overset{H}{|}}{\underset{\underset{CH_3}{|}}{C}}$—$CH_2\overset{\overset{O}{\|}}{C}CH_3$

6. $C_6H_{12}O_2$ IR: 1740   ester

^{13}C NMR: 175 (s), 65 (q), 42 (t), 37 (d), 18 (q)

$C_6H_{12}O_2$

6H

1H

2H

3H

$$CH_3OCCH_2CH \begin{matrix} CH_3 \\ | \\ CH_3 \end{matrix}$$

(with O double bonded to C)

4

7. C_5H_9OCl IR: 1710

EU= 1   C=O

C_5H_9OCl

2H   1H   3H   3H

(NMR spectrum with peaks at ~3 ppm and ~2 ppm)

Structure 1 (boxed):

$$CH_3-\underset{\underset{Cl}{\overset{|}{CH_2}}}{\overset{\overset{H}{|}}{C}}-\overset{\overset{O}{\|}}{C}CH_3$$

Structure 2:

$$CH_3\overset{\overset{O}{\|}}{C}CH_2\underset{\underset{Cl}{|}}{\overset{\overset{H}{|}}{C}}CH_3$$
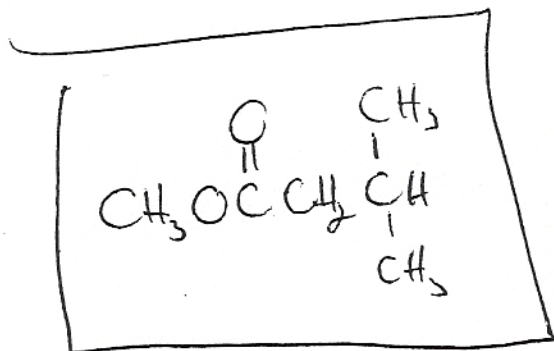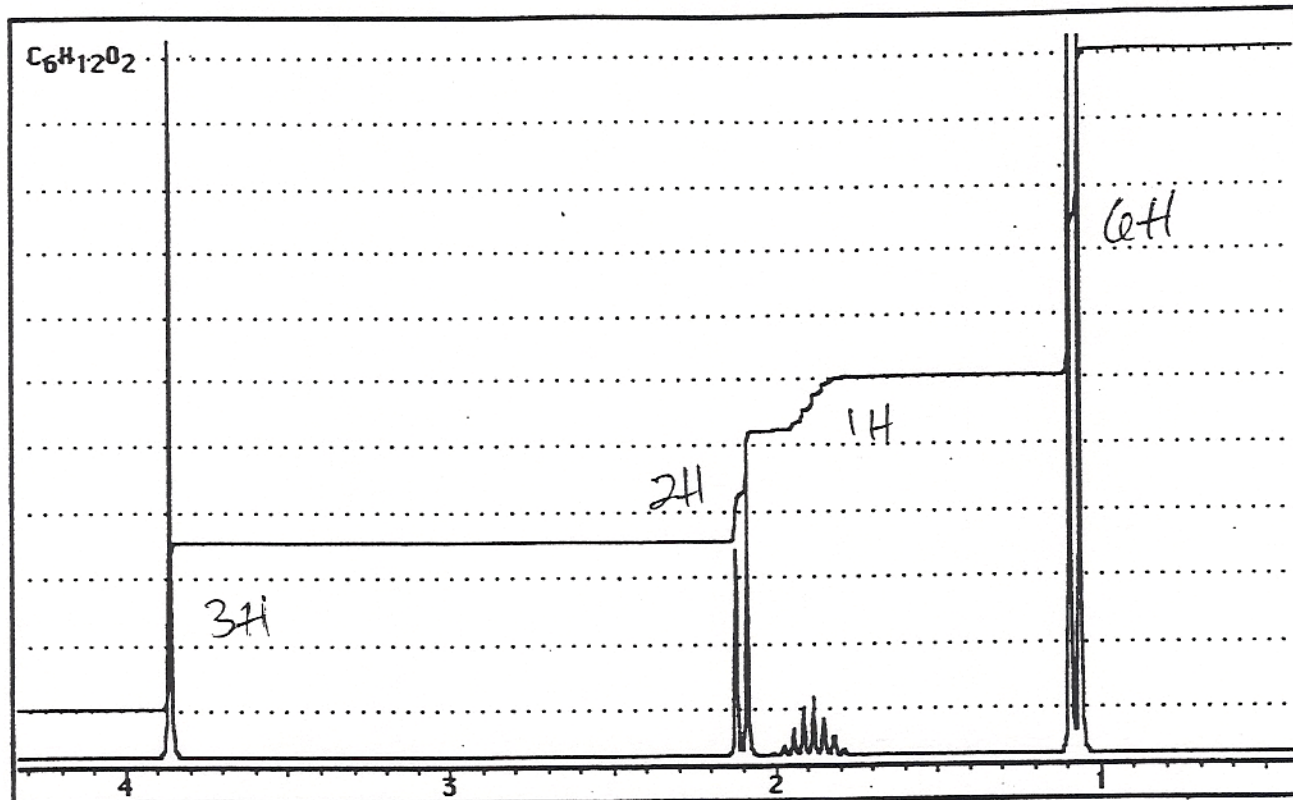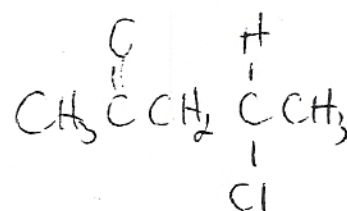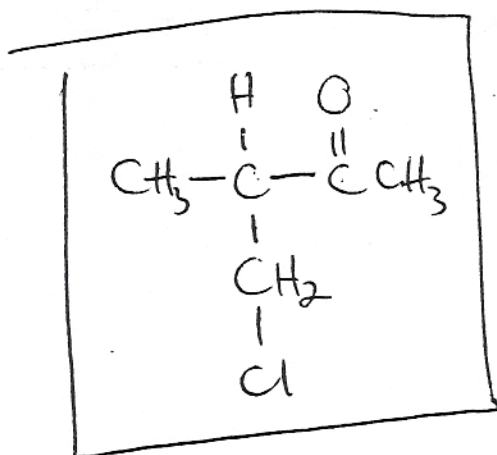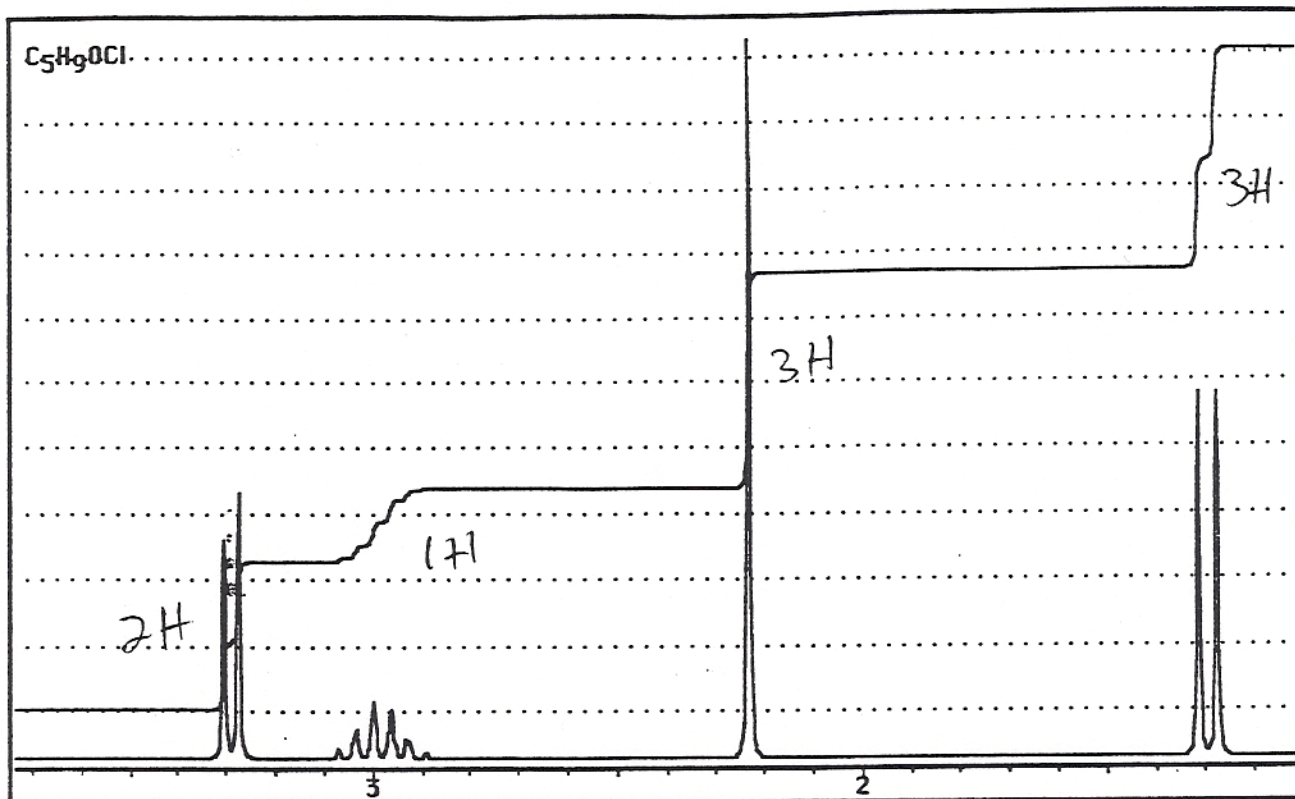
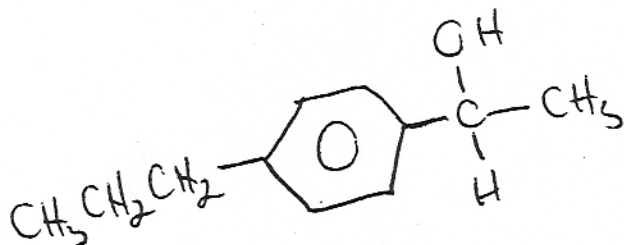close, but poorer for chemical shift. partial credit.

8. $C_{11}H_{16}O$ IR: 3300-3200   OH

^{13}C NMR: 148 (s), 144 (s), 133 (d), 124 (d), 80 (d), 42 (t), 35 (t), 30 (q), 20 (q)

EU=4

$C_{11}H_{16}O$

4H   1H   1H   2H   2H   3H   3H

7   6   5   4   3   2   1

$CH_3CH_2CH_2$ — [benzene ring with O] — C(OH)(H) — CH_3

6
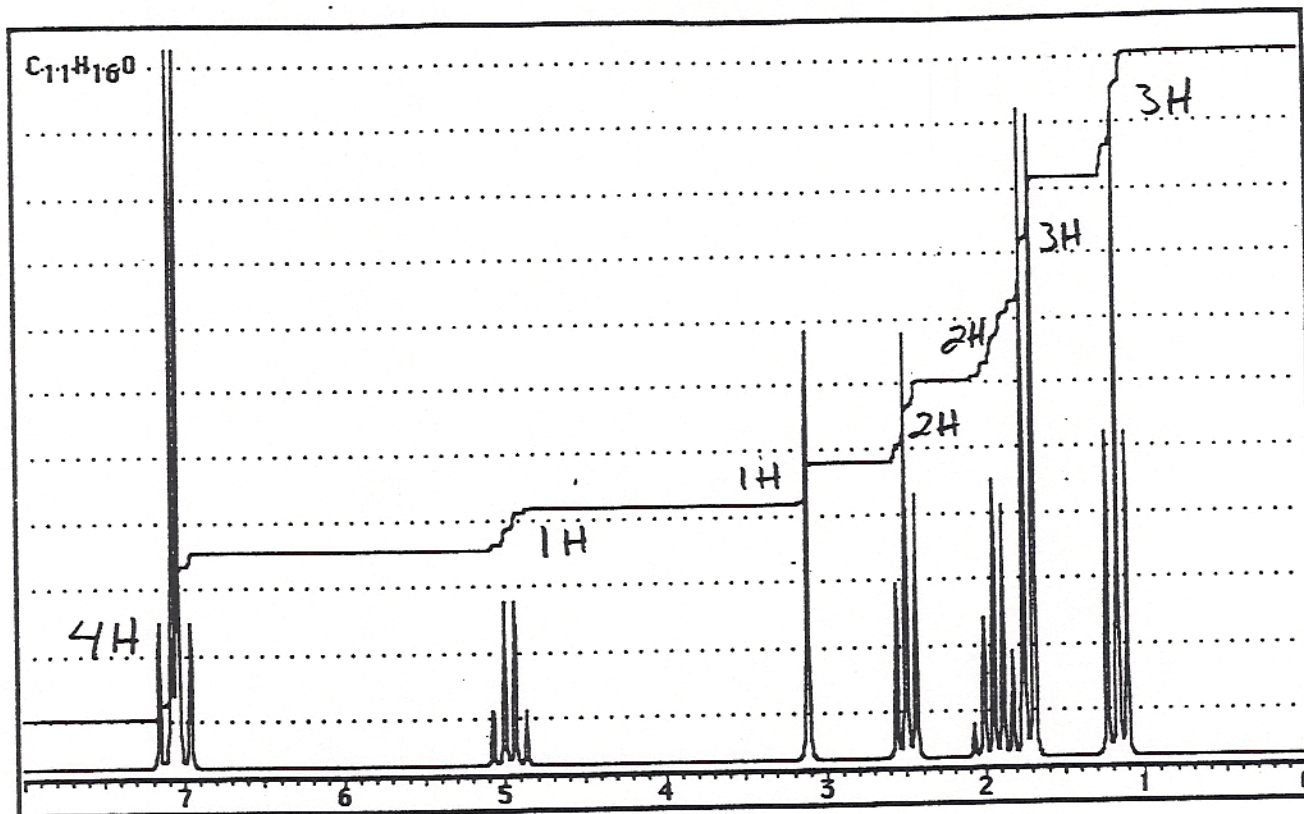
9. $C_5H_{12}O$

Carbon 13 NMR

$$CH_3-\overset{\overset{\displaystyle CH_3}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-CH_2-CH_2OH$$
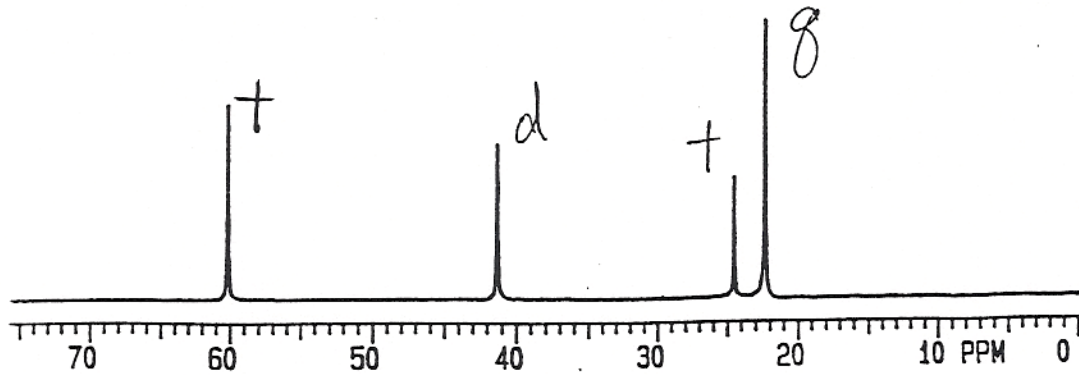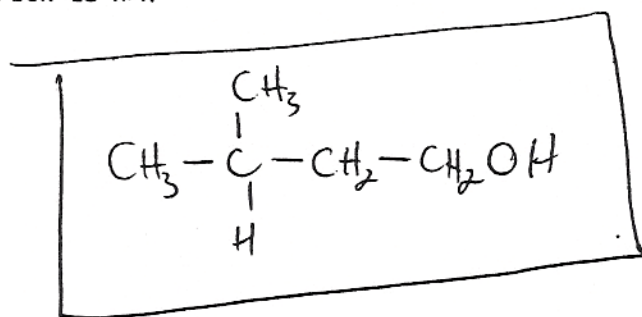
10. $C_4H_7BrO_2$ IR: 3300-2500, 1710

3H, t, 1.08
2H, multiplet, 1.89
1H, t, 4.23
1H, s (broad), 10.97

$$CH_3CH_2 - \underset{\underset{Br}{|}}{CH} - \overset{\overset{O}{\|}}{C}OH$$