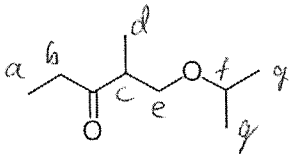
Chem 342 Jasperse Test 2 Version 2 Name:

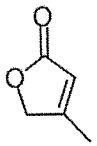
NMR, IR

1. Predict the ^1H 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.



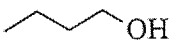
a 1's 3H t
b 2's 2H q
c 2's 1H m
d 1's 3H d
e 3's 2H d
f 3's 1H m
g 1's 6H d

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).

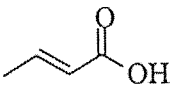


220-160 s
160-100 d
160-100 s
100-50 t
50-0 q

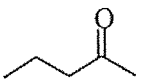
3. Match the following structures with the listed feature IR signals.



A 1710 C



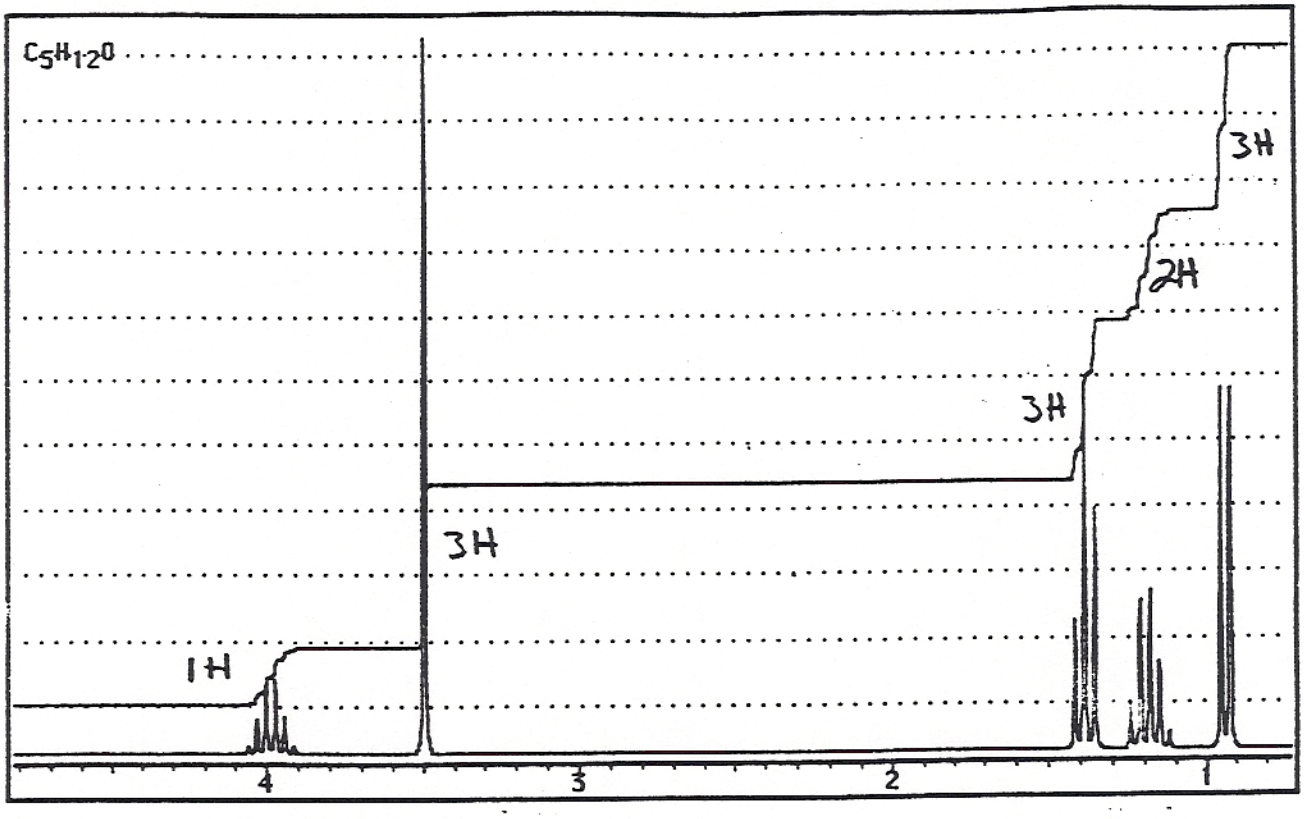
B 3300-3400 A

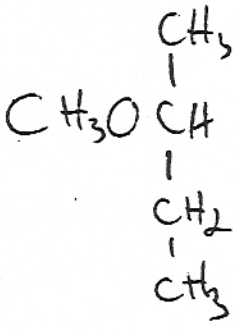


C 1680, 3300-2500 B

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

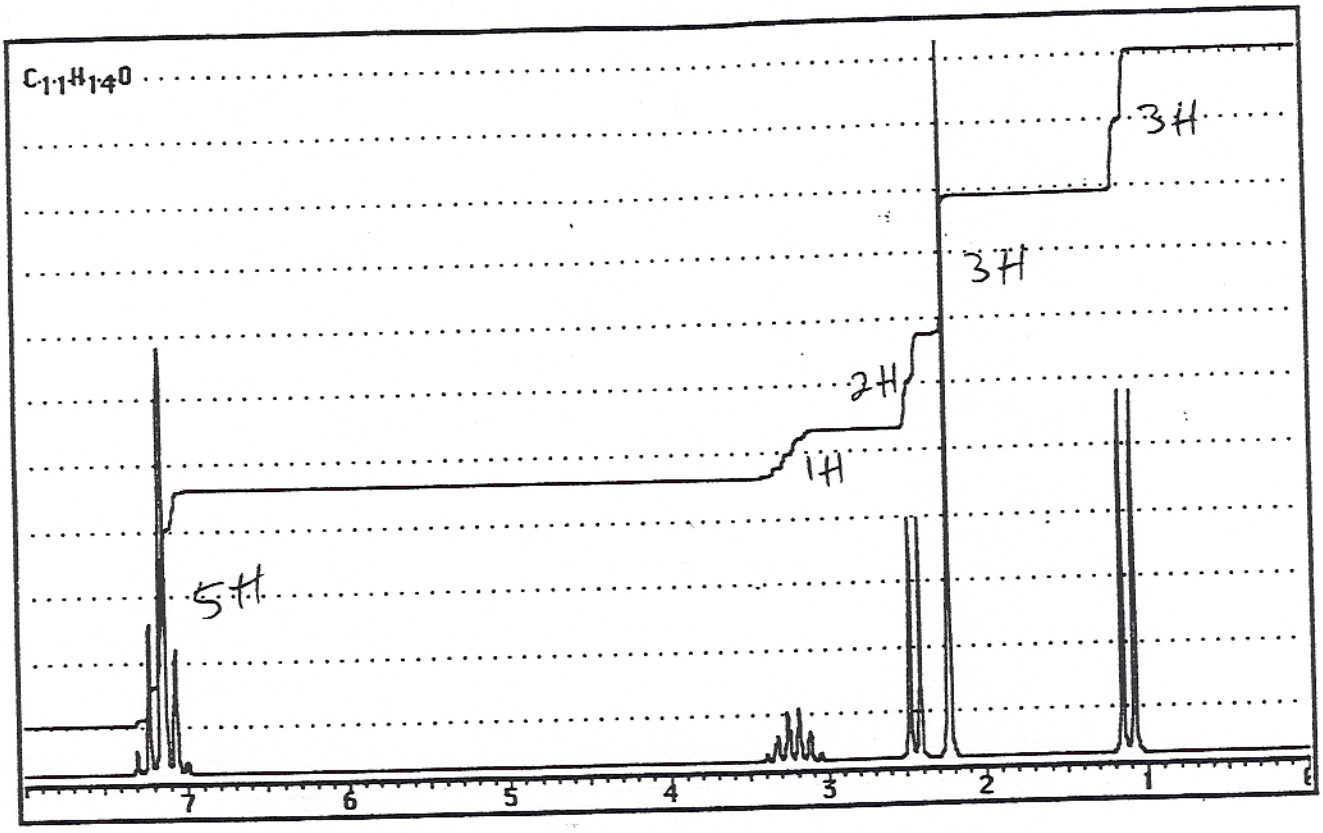


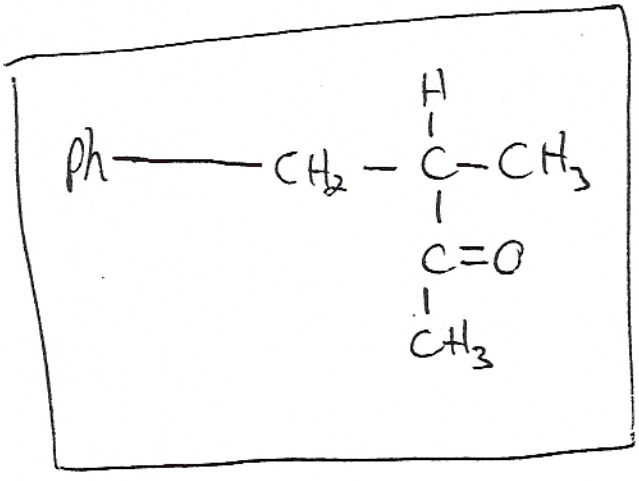


5. $C_{11}H_{14}O$ IR: 1710 C=O, not conjugated error (+)

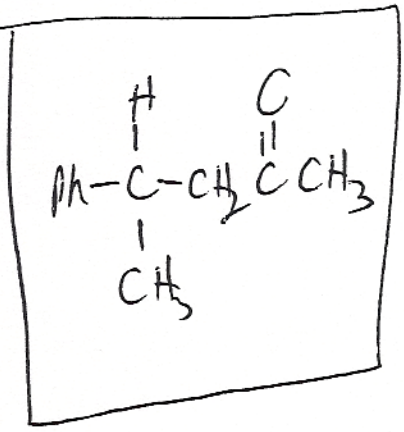
^{13}C NMR: 202 (s), 152 (s), 134 (d), 127 (d), 122 (d), 42 (d), 35 (q), 20 (q)

EU = 5



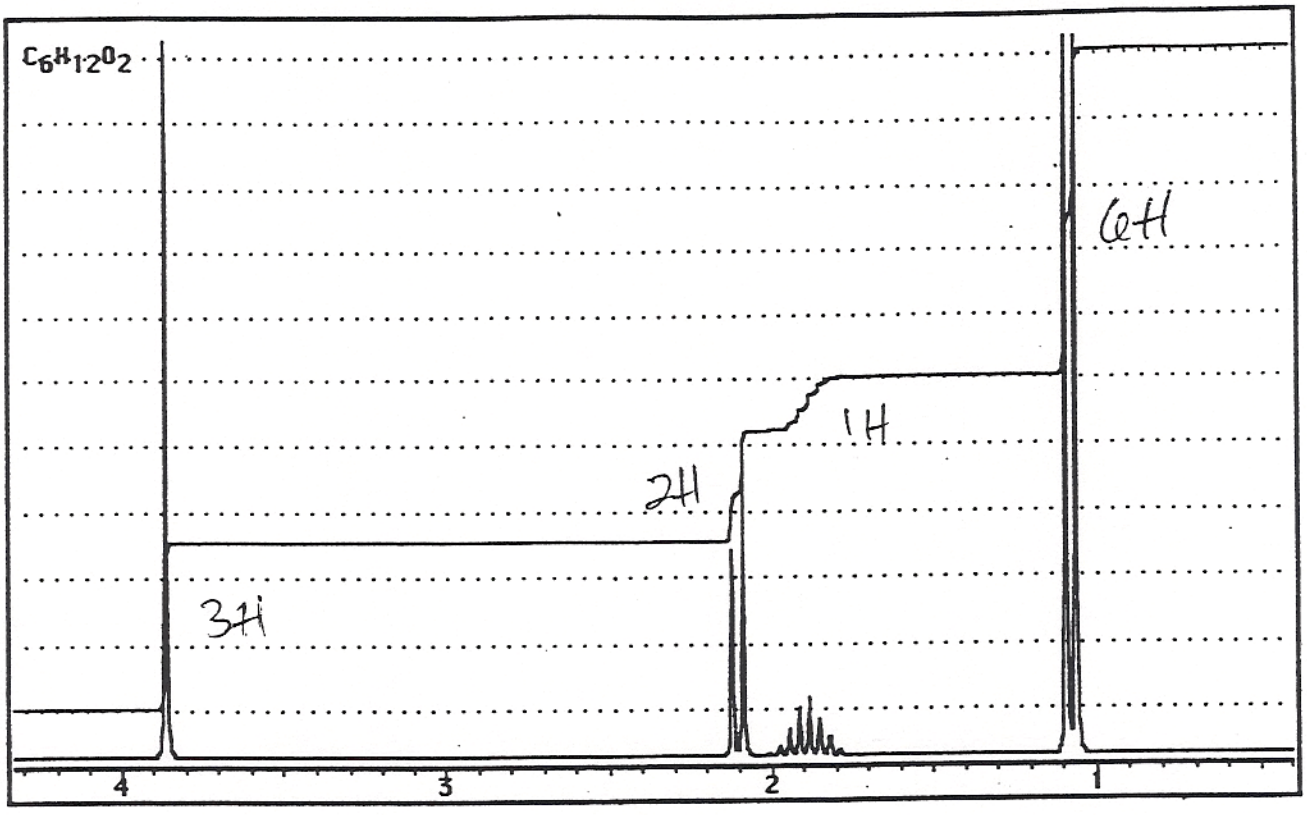


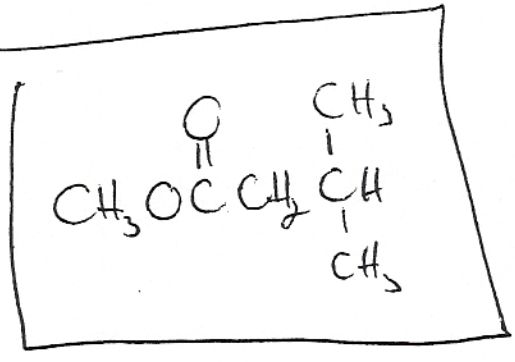
or



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

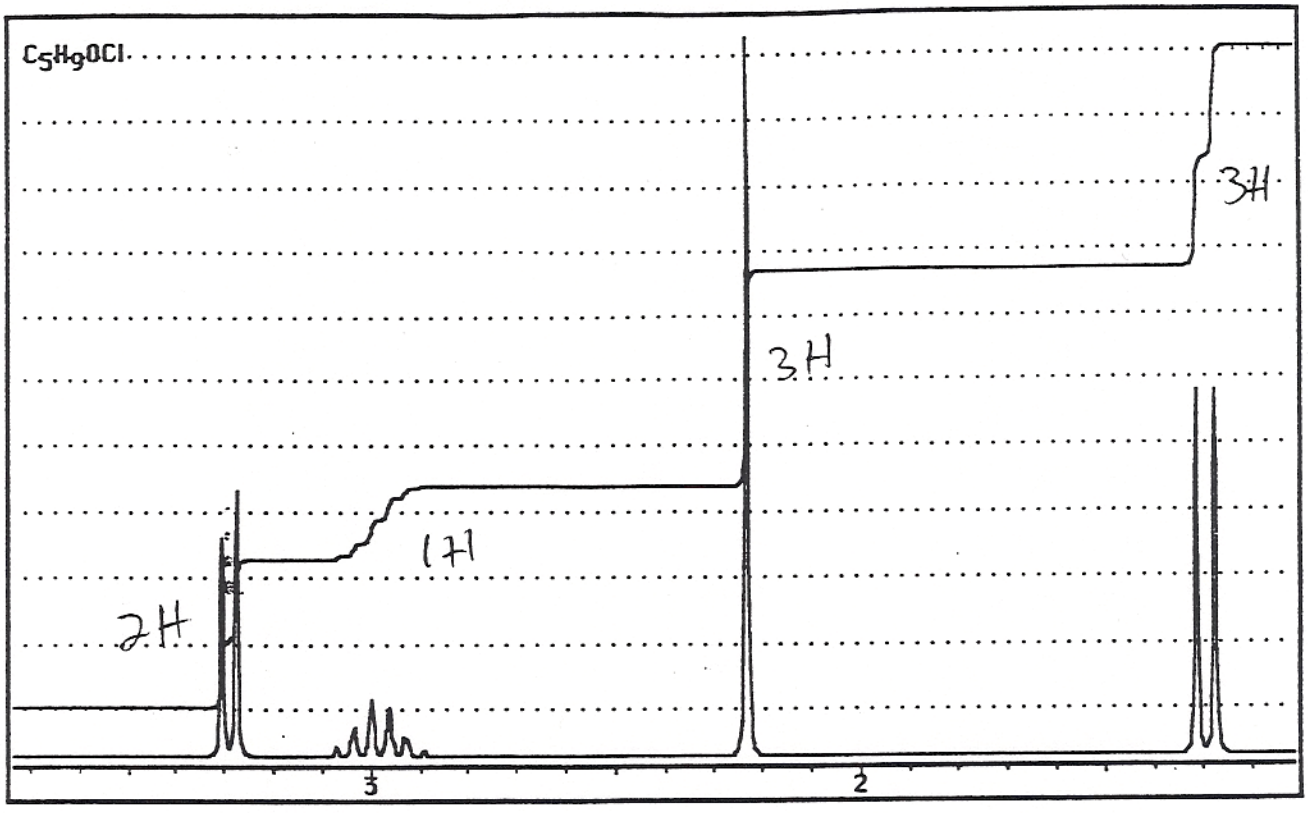
^{13}C NMR: 175 (s), 65 (q), 42 (t), 37 (d), 18 (q)

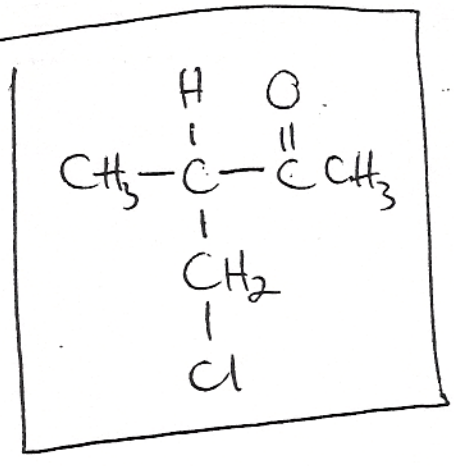


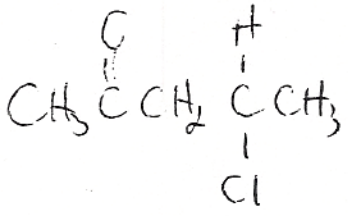


7. C_5H_9OCl IR: 1710

EU=1 C=O





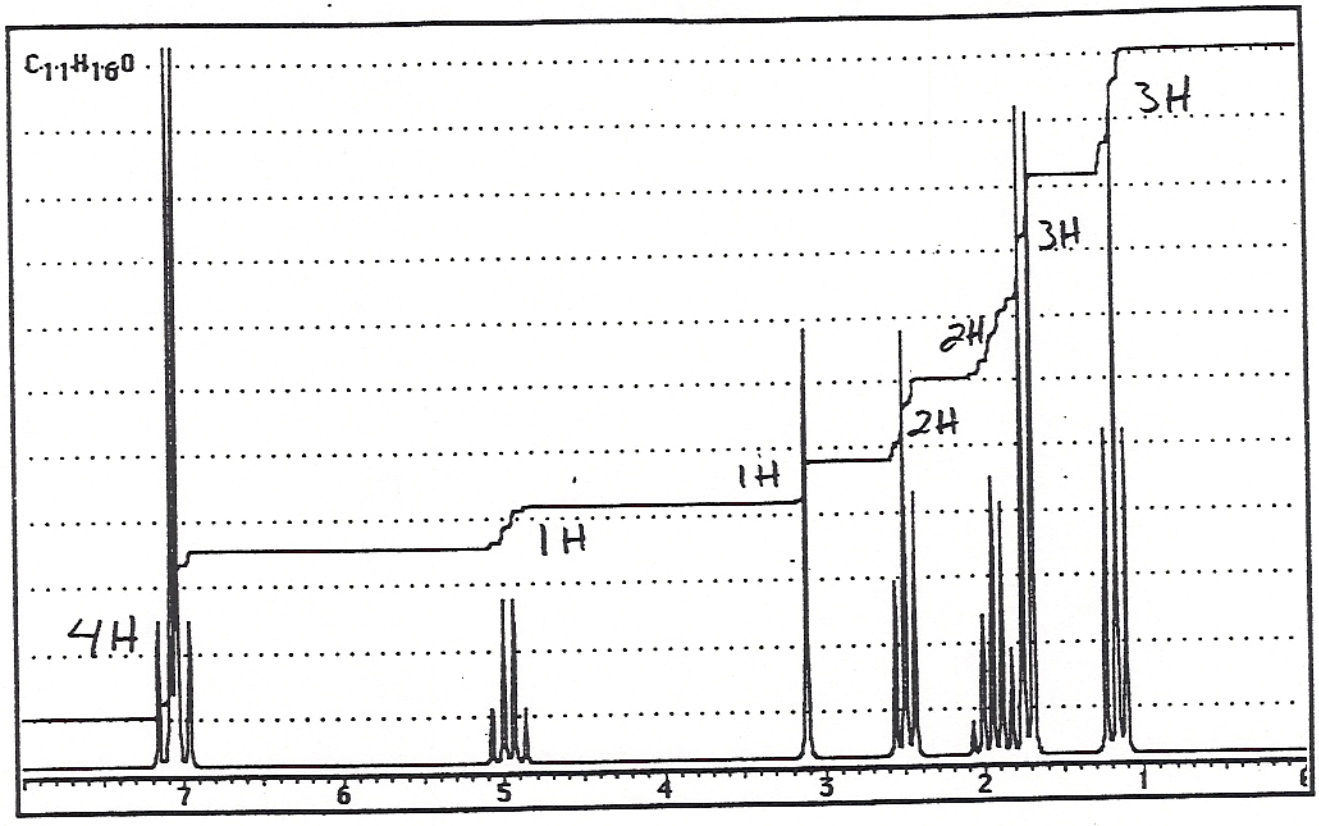


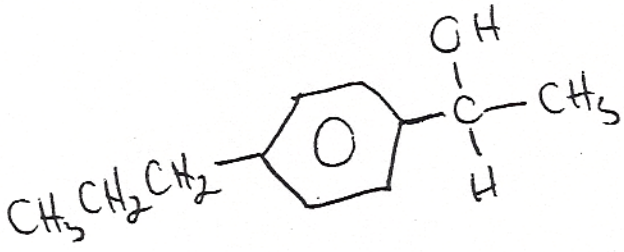
close, but poorer for chemical shift. Partial credit.

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

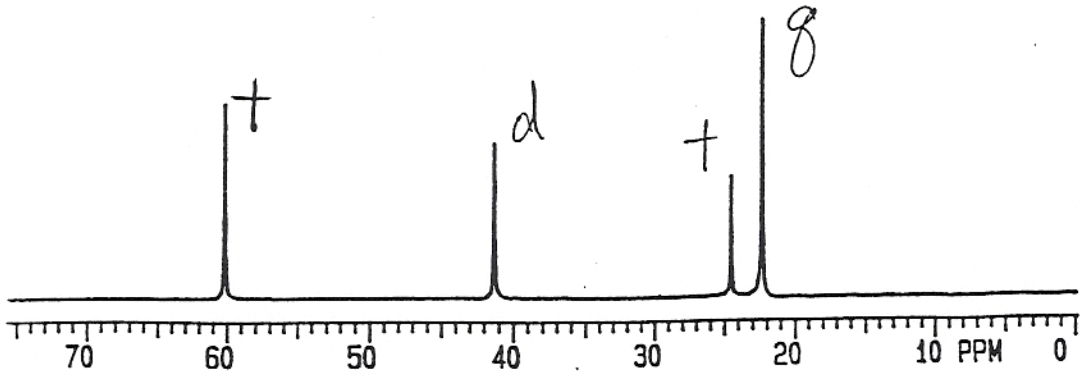
^{13}C NMR: 148 (s), 144 (s), 133 (d), 124 (d), 80 (d), 42 (t), 35 (t), 30 (q), 20 (q)

EW=4

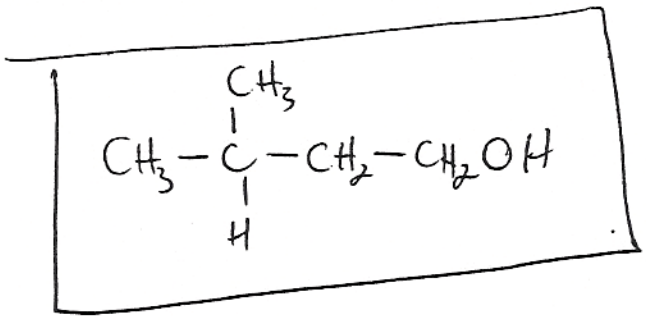




9. $C_5H_{12}O$



Carbon 13 NMR



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