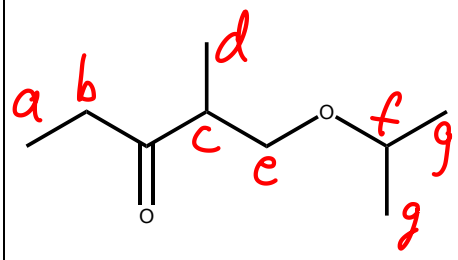
V2 Answers

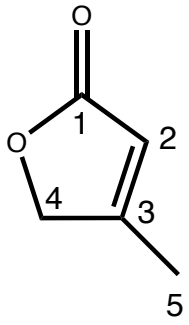
Chem 360-Jasperse Test #2 NMR, IR Version 2

1. Predict the ^{1}H NMR spectrum. Include the source (CH_3-1, etc); approximate chemical shifts (1's, 2's, etc.); integration (1H, 2H, etc.); and splitting (either list the number of lines, or else use letters: "s" for singlet; "d" for doublet etc.). If signals are symmetry equivalent, do not list them twice.



Source	Chem Shift	Integration	Splitting
CH_3-a	1's	3H	3 = t
CH_2-b	2's	2H	4 q
CH-c	2's	1H	6 mult.
CH_3-d	1's	3H	2 d
CH_2-e	3's	2H	2 d
CH-f	3's	1H	7 mult.
CH_3-g	1's	6H	2 d

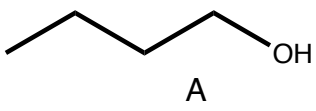
2. Predict the ^{13}C NMR spectrum. Include the approximate chemical shifts (220-160, 160-100, 100-50, or 50-0) and the splitting if a coupled carbon NMR was taken (can either use letters, q, t, d, s, or else number of lines).



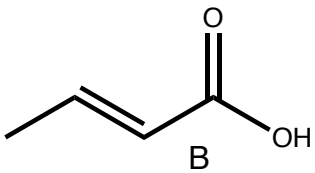
Source	Approximate Chem Shift	Splitting
C1	220-160	s
C2	160-100	d
C3	160-100	s
C4	100-50	t
C5	50-0	q

3. Match the following structures with the listed feature IR signals. (Write the letter of the structure by the IR signal):

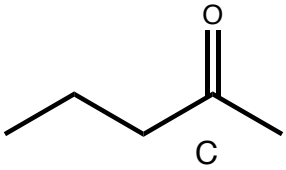
1) 1710 C 2) 3300-3400 A 3) 1680, 3300-2200 B



A



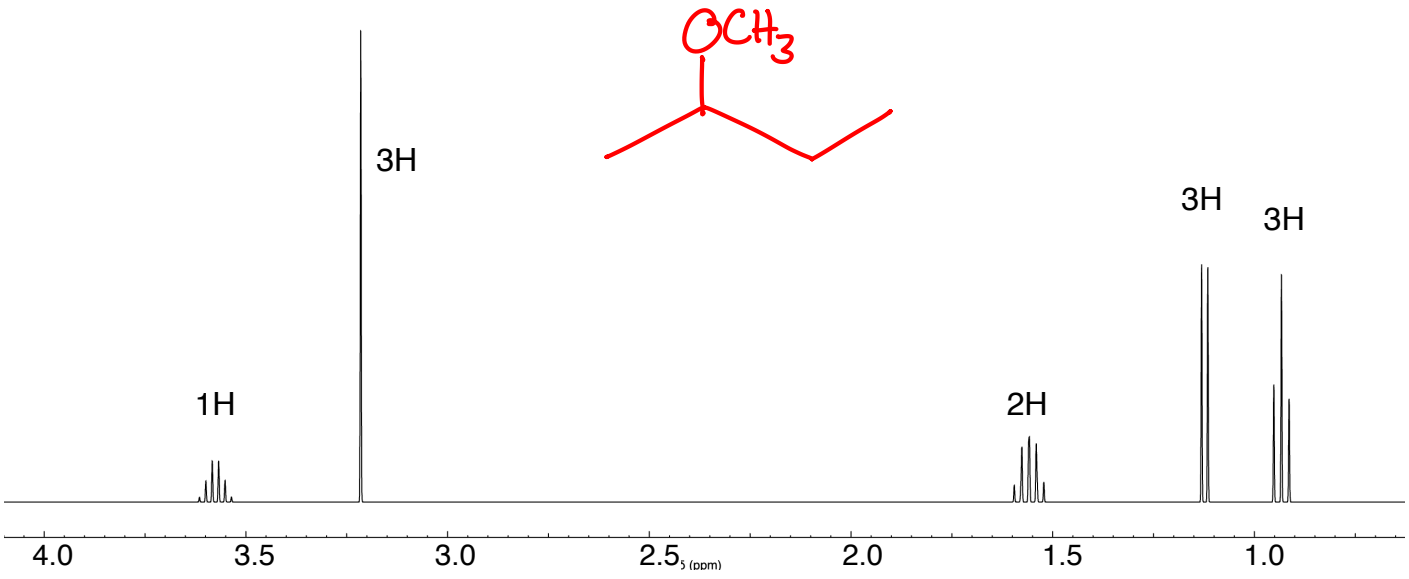
B



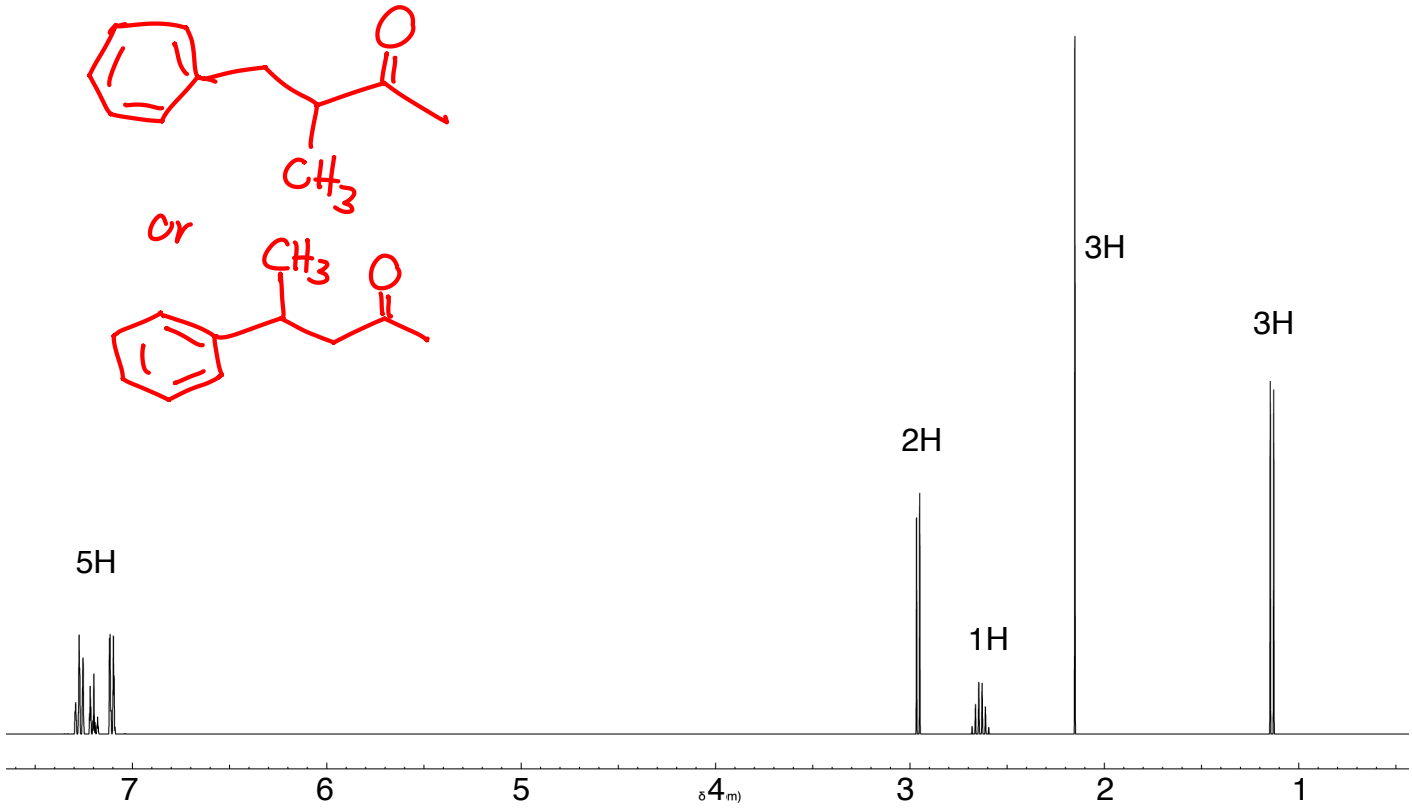
C

For the remainder of the test, 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 you work, make a structure, or tell me what you know for sure.

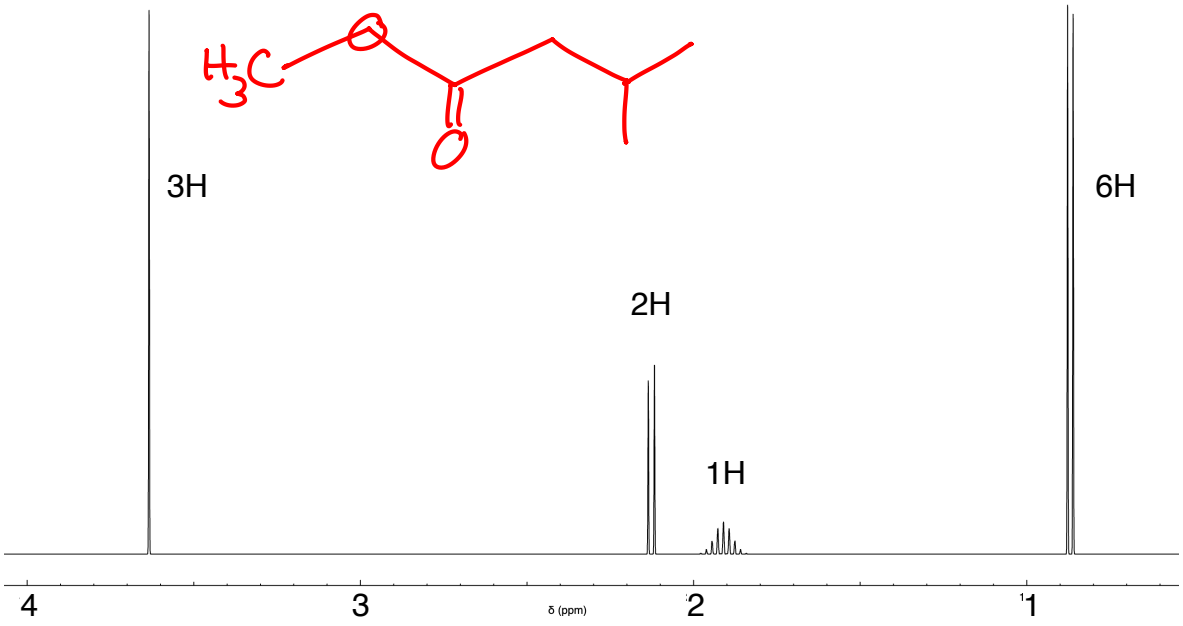
4. $C_5H_{12}O$ IR: Nothing interesting



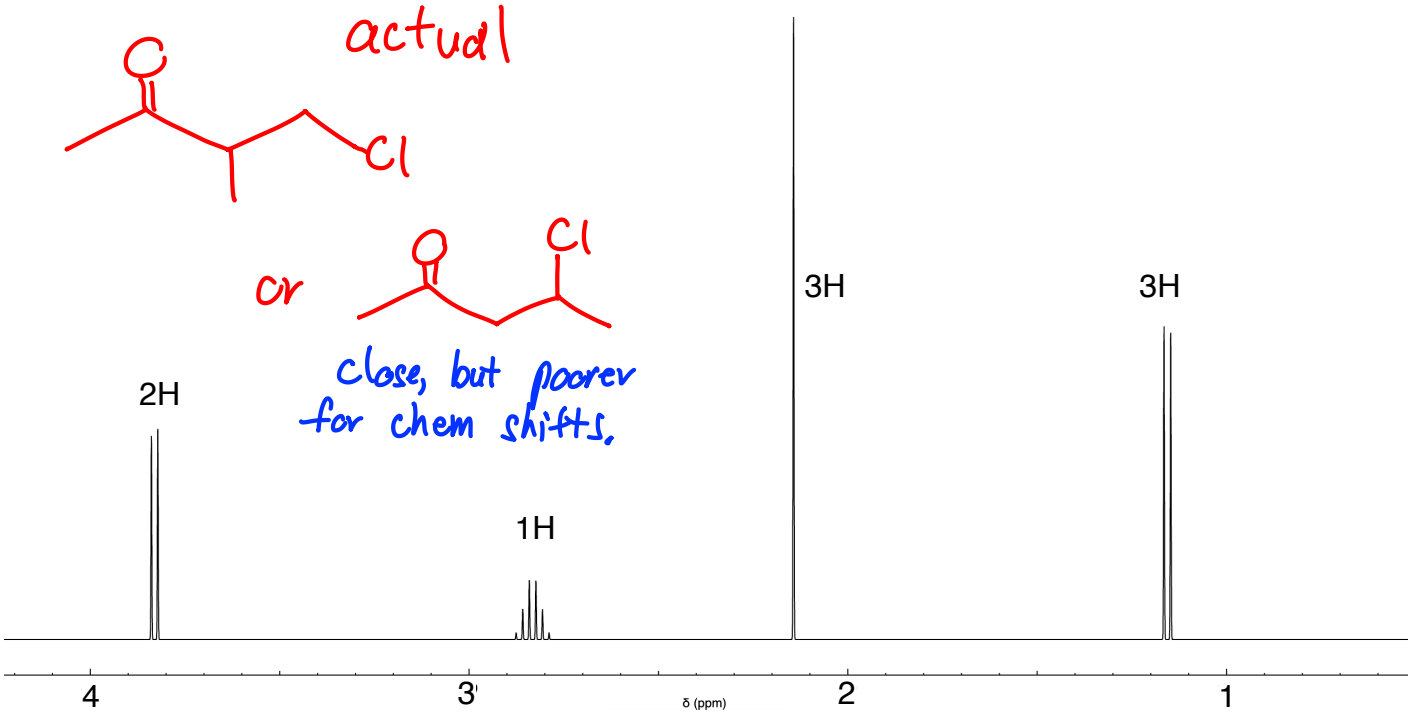
5. $C_{11}H_{14}O$ IR: 1710 ^{13}C: 211 (s), 139 (s), 134 (d), 127 (d), 122 (d), 42 (d), 35 (t), 20 (q), 15 (q)
   - (Note: There are two plausible solutions to this problem)



6. $C_6H_{12}O_2$ IR: 1745
^{13}C: 170 (s), 65 (q), 42 (t), 37 (d), 18 (q)

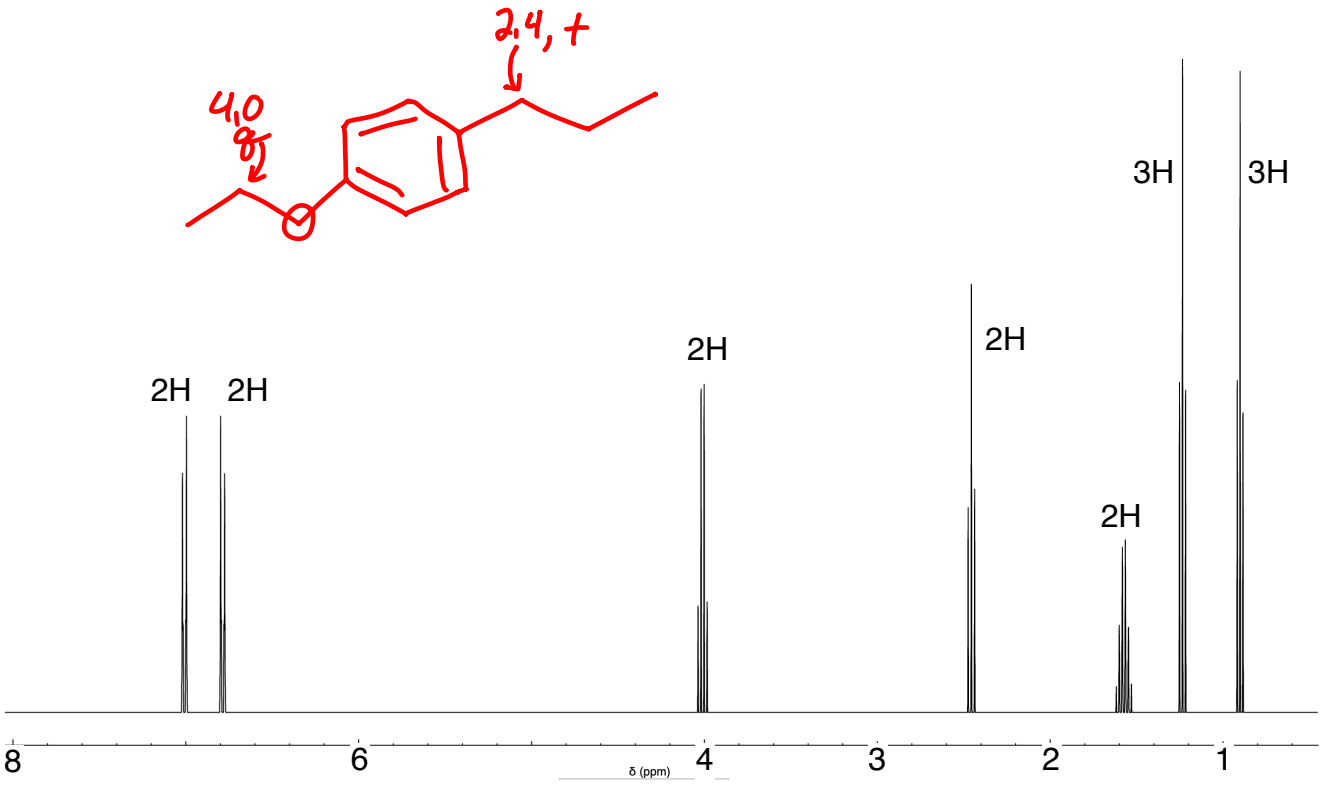


7. C_5H_9OCl IR: 1710



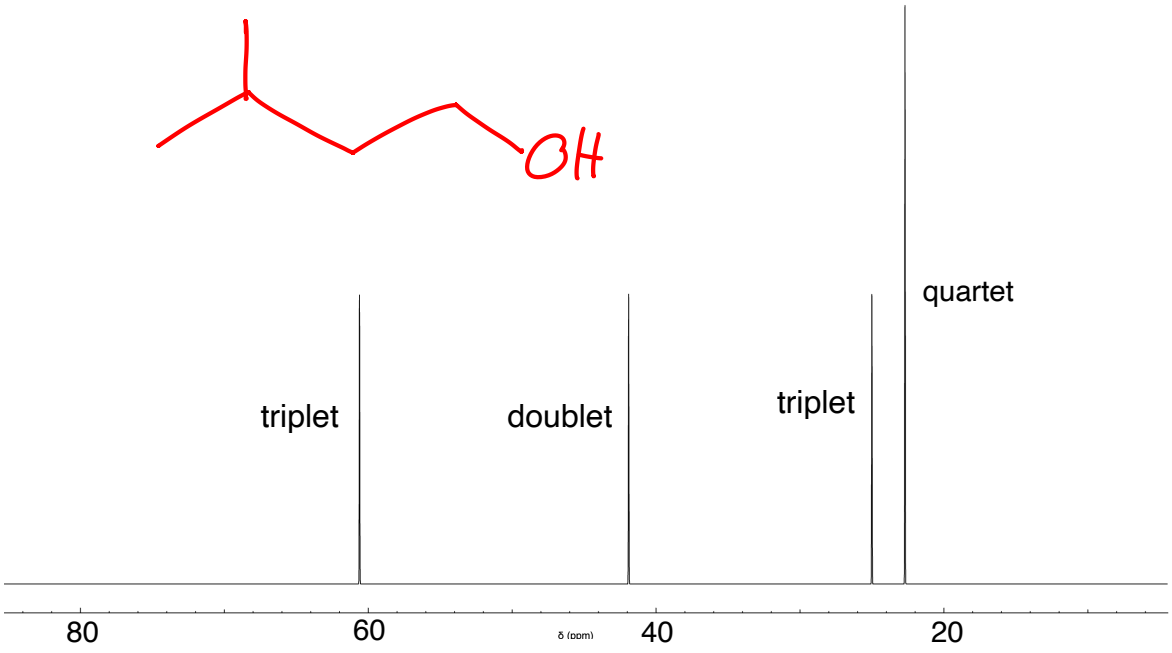
8. $C_{11}H_{16}O$ IR: Nothing interesting

^{13}C: 148 (s), 140 (s), 130 (d), 125 (d), 64 (t), 38 (t), 25 (t), 15 (q), 14 (q)

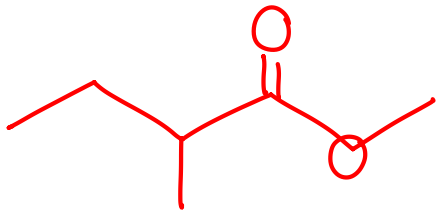


9. $C_5H_{12}O$

- The spectrum displayed is a "decoupled" 13-C NMR spectrum. (No splitting)
- But beside each coupled peak is a label that tells whether the carbon would be a singlet, doublet, triplet, or quartet **if** a "coupled" 13-C NMR had been obtained.



10. $C_6H_{12}O_2$ IR: 1745



0.92, 3H, triplet
1.12, 3H, doublet
1.54, 2H, pentet
2.38, 1H, sextet
3.89, 3H, s

- I have not, accidentally or intentionally, seen copies or parts of the test in advance, including online. In the event that I did, I will report this to the instructor as soon as possible.