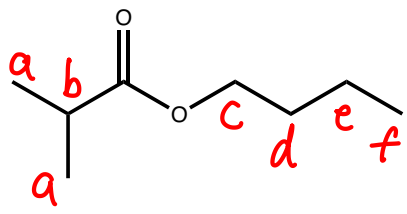
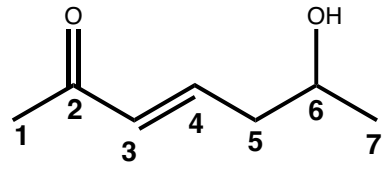
Chem 360-Jasperse Test #2 NMR, IR Version 1 **V1 Answers**

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	# lines
CH_3-a	1's	6H	d	2
CH-b	2's	1H	septet	7
CH_2-c	3's (low 4's)	2H	+	3
CH_2-d	1's	2H	pentet	5
CH_2-e	1's	2H	sextet	6
CH_3-f	1's	3H	+	3

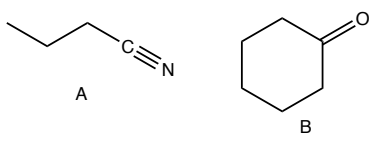
2. Predict the ^{13}C NMR spectrum. Include the approximate chemical shifts (220-160, 160-100, 100-50, or 50-0) and the splitting if a coupled carbon NMR was taken (can either use letters, q, t, d, s, or else number of lines).



Source	Approximate Chem Shift	Splitting
C1	50-0	q
C2	220-160	+
C3	160-100	d
C4	160-100	d
C5	50-0	+
C6	100-50	d
C7	50-0	q

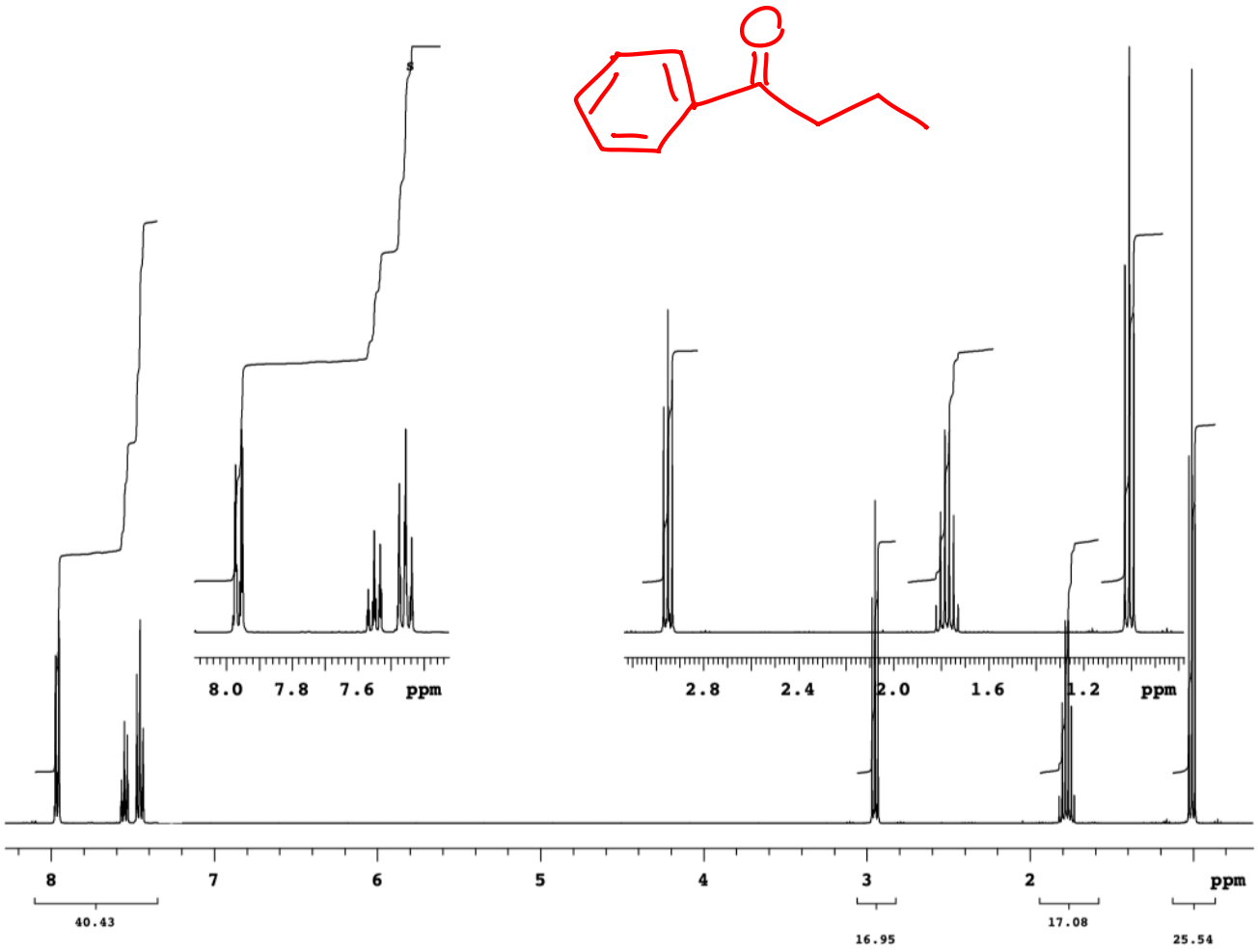
3. Match the following structures with the listed feature IR signals. (Write the letter of the structure by the IR signal):

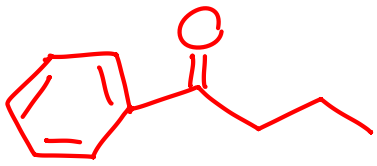
1) 3300-3400 D 2) 3300-2500, 1680 C 3) 2200 A 4) 1710 B



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. $C_{10}H_{12}O$ IR: 1670
^{13}C NMR: 210 (s, short), 150 (s, short), 130 (d, tall), 124 (d, tall), 120 (d), 33 (t), 26 (t), 20 (q)



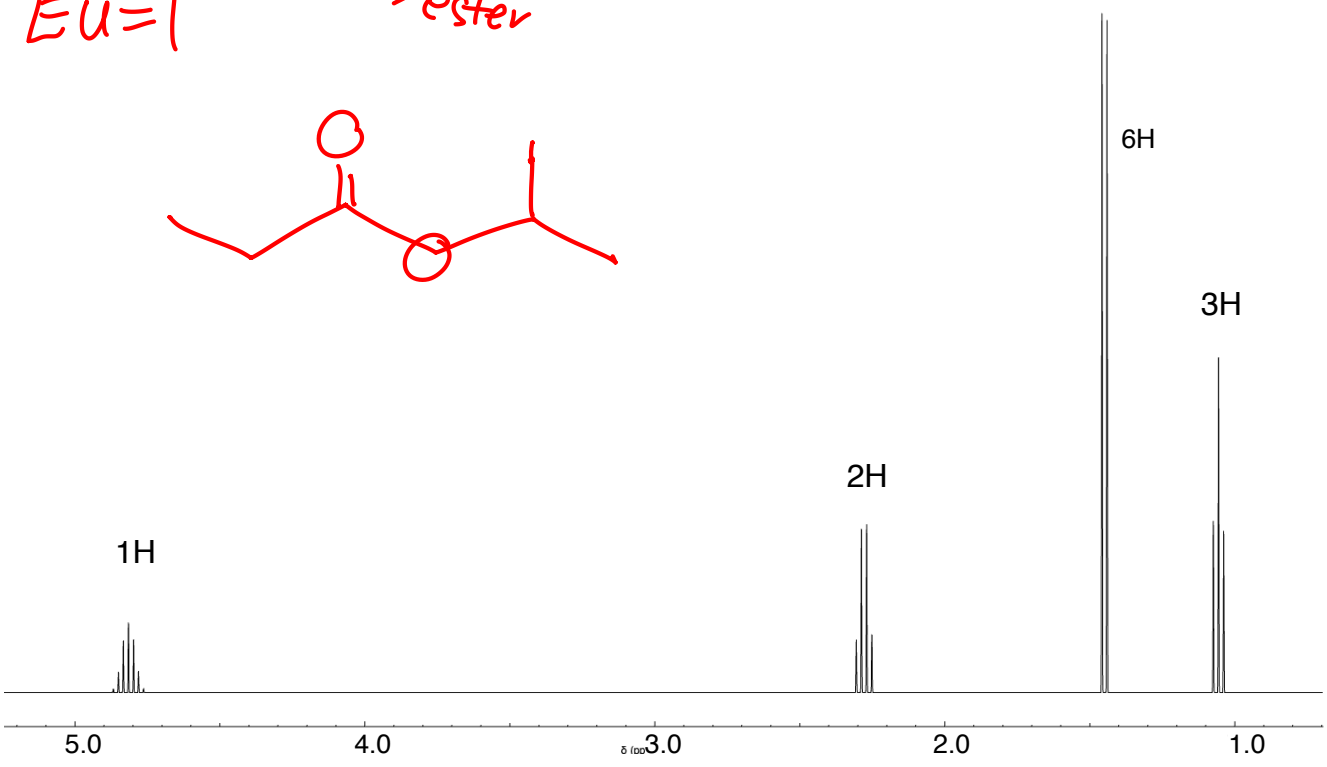


EU = 5 ⇒ aromatic + C=O
IR 1670 ⇒ C=O conjugated
5H integration in 7's ⇒ mono-subbed aromatic

5. $C_6H_{12}O_2$ IR: 1745 ^{13}C: 180 (s), 70 (d), 36 (t), 30 (q), 20 (q, tall)

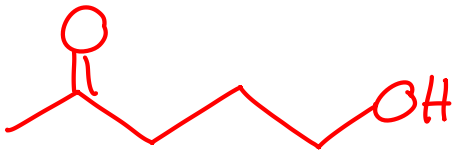
EU=1

⇒ ester



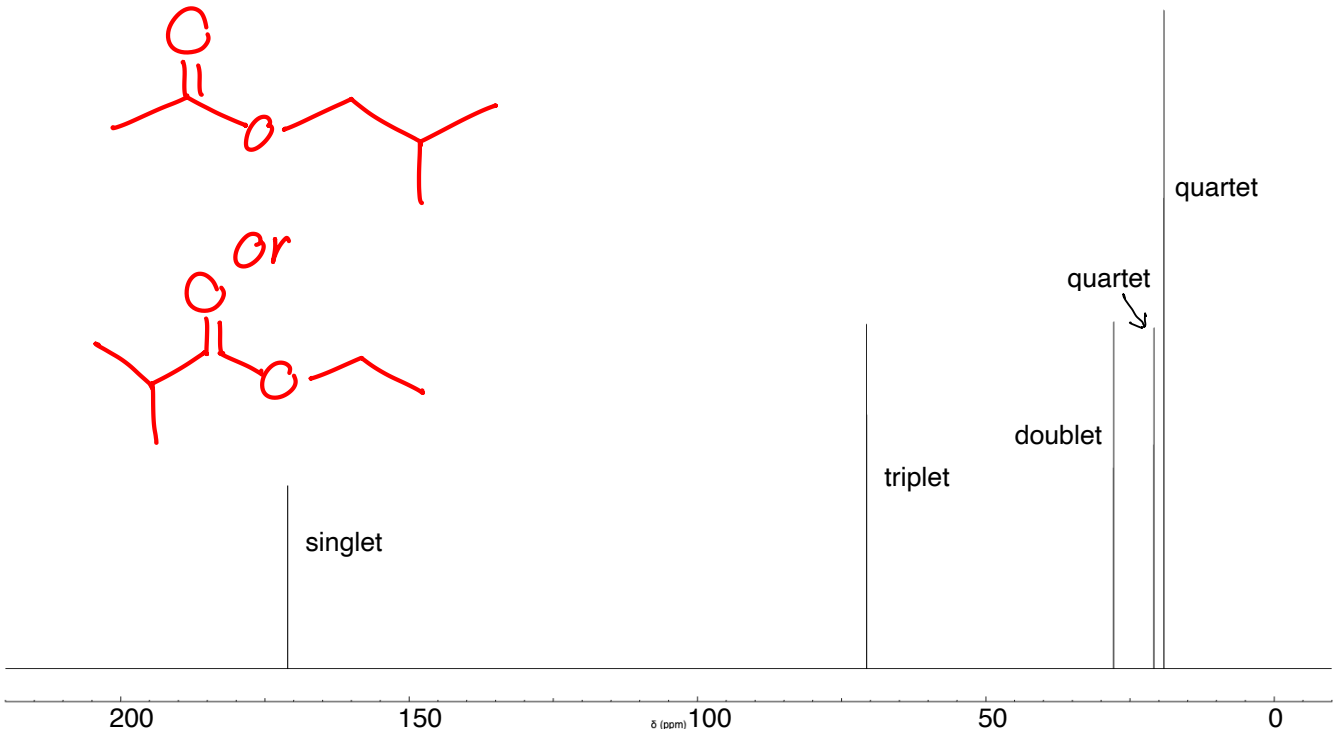
6. $C_5H_{10}O_2$ IR: 3300-3200, 1710 ⇒ alcohol ⇒ ketone

^{13}C: 210 (s), 65 (t), 38 (t), 35 (t), 28 (q)

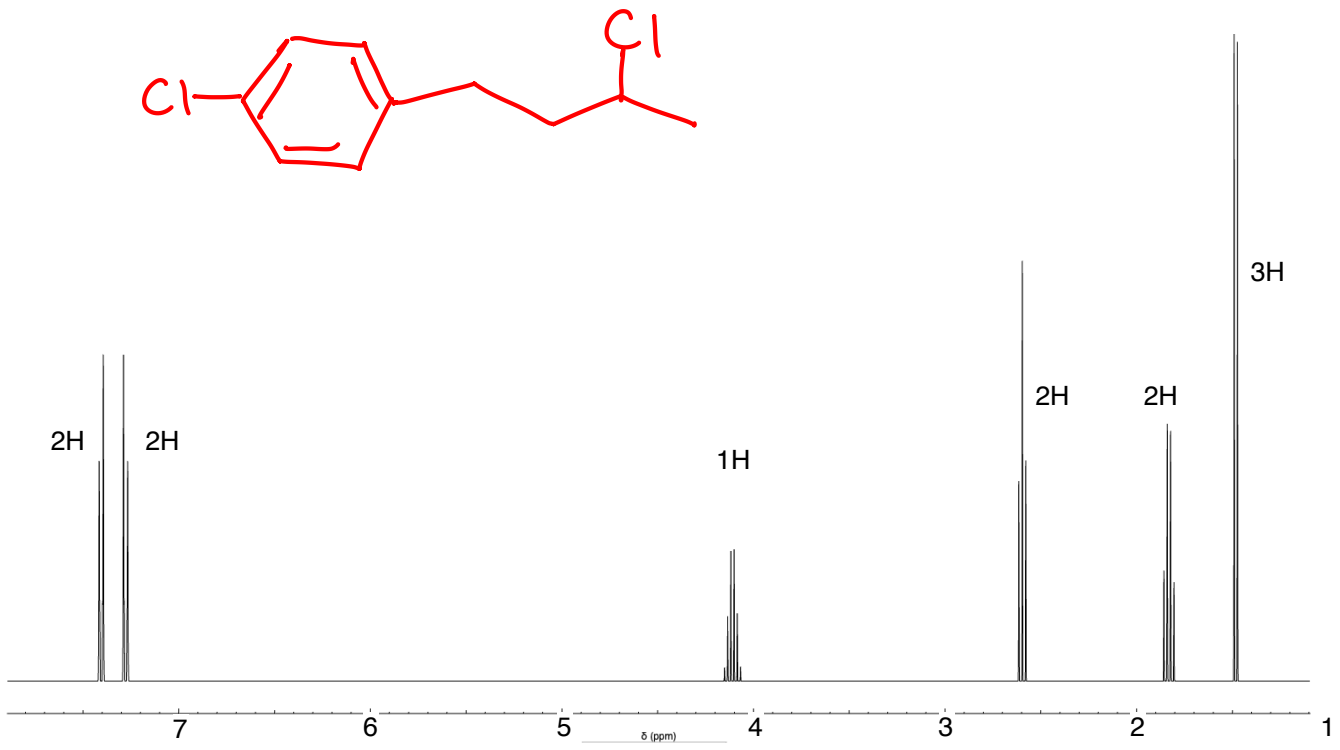


7. $C_6H_{12}O_2$ IR: 1745

- 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.
- (Note: There are two plausible solutions to this problem)



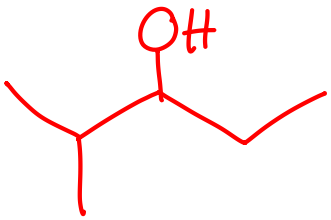
8. $C_{10}H_{12}Cl_2$ ^{13}C: 150 (s), 144 (s), 133 (d), 126 (d), 58 (d), 37 (t), 32 (t), 22 (q)



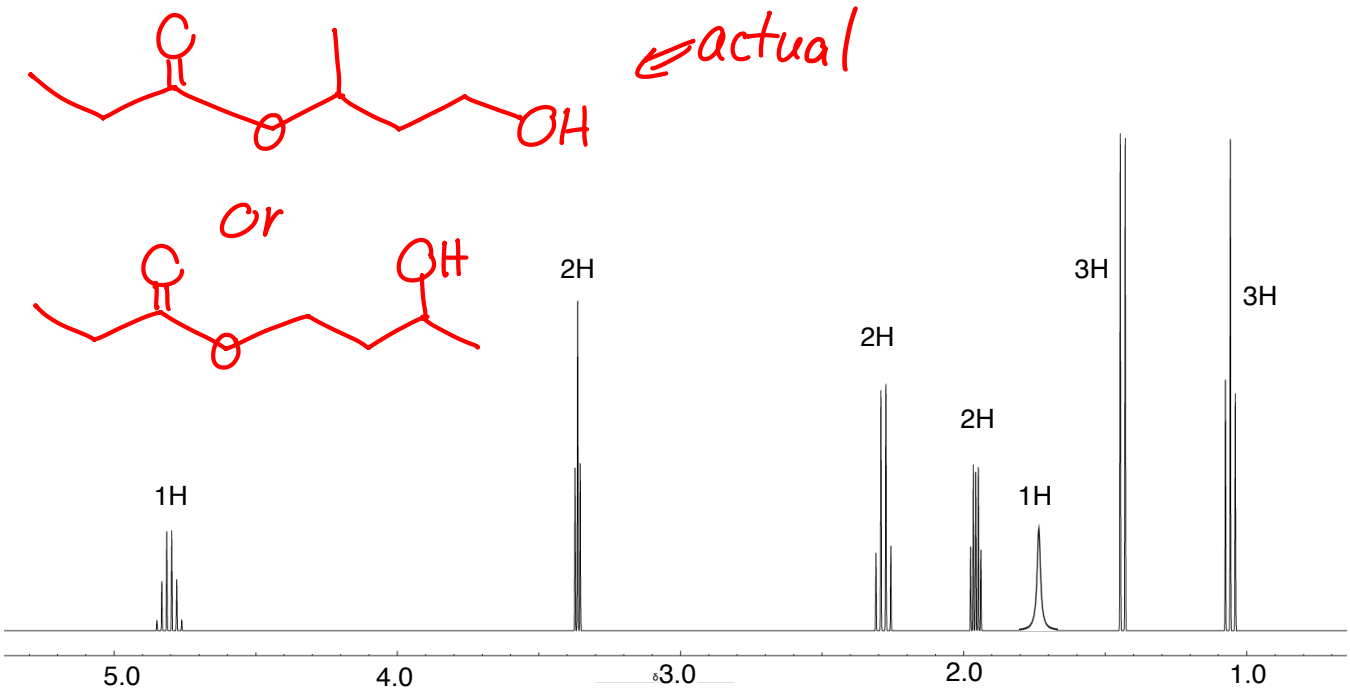
9. $C_6H_{14}O$

IR: 3300-3200
13C NMR: 78 (d), 40 (d), 36 (t), 25 (q), 20 (q, extra tall)

6H, d, 1.0
3H, t, 1.2
2H, pentet, 1.4
1H, octet, 1.8
1H, broad s, 3.0
1H, q, 3.8



10. $C_7H_{14}O_3$ IR: 3300-3200, 1745
13C-NMR: 180 (s), 75 (d), 65 (t), 38 (t), 30 (t), 25 (q), 20 (q)
Either of 2 answers will be accepted for this question.



- 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.