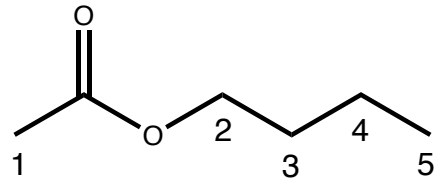
V4 Answers 1

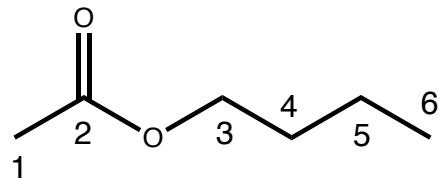
Chem 360-Jasperse Test #2 NMR, IR Version 4.

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_3-1	2's	3H	1 = s
CH_2-2	3's	2H	3 +
CH_2-3	1's	2H	5 pentet
CH_2-4	1's	2H	6 sextet or m
CH_3-5	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).



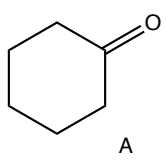
Source	Approximate Chem Shift	Splitting
C1	50-0	q
C2	220-160	s
C3	100-50	+
C4	50-0	+
C5	50-0	+
C6	50-0	q

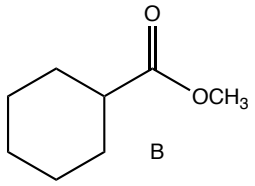
3. Match the following structures A, B, and C with the listed feature IR signals.

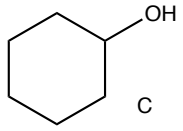
1) 3300-3400 C

2) 1745 B

3) 1710 A





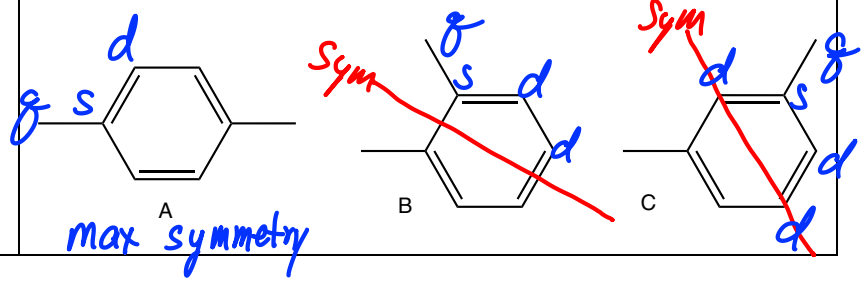


4. Match the dimethyl benzene isomer for which the ^{13}C NMR spectrum has:.

1) 3 signals (q, s, d) A

2) 4 signals (q, s, d, d) B

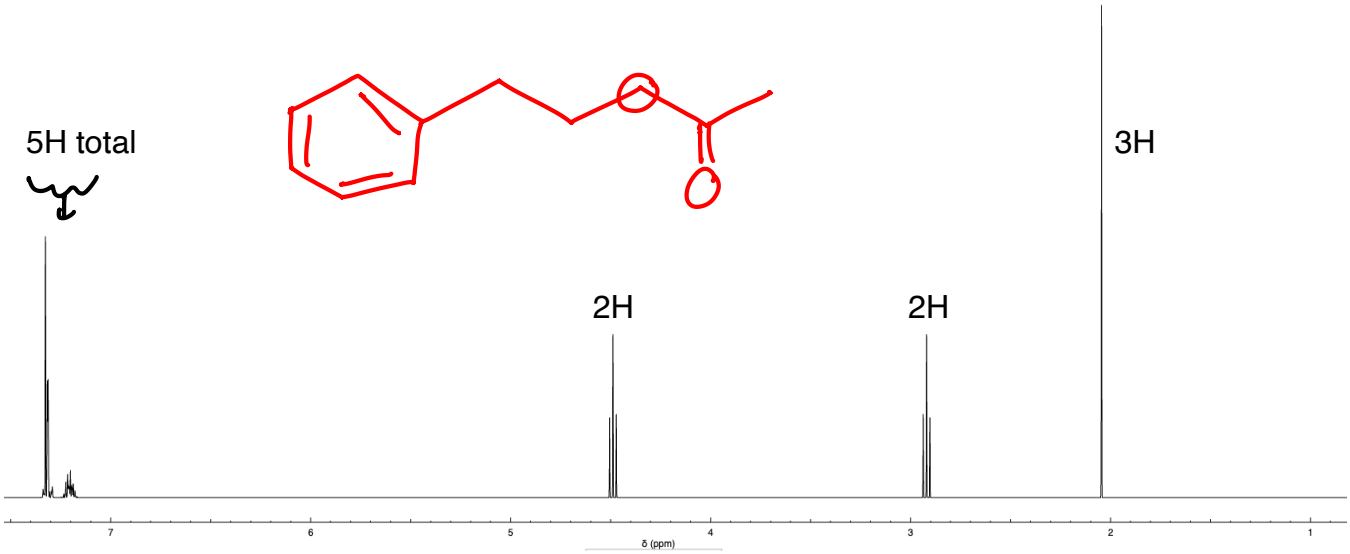
3) 5 signals (q, s, d, d, d) C



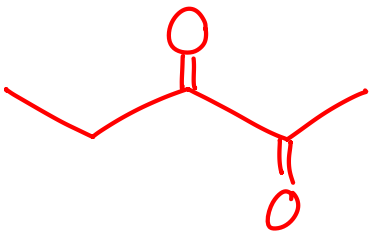
For the remainder of the test, solve the structures for the following. If you get a structure perfect, you will get full credit. If you do not get a structure perfect, you may still get some partial credit. Thus, it is in your interest to show some of you work, make a structure, or tell me what you know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

5. $C_{10}H_{12}O_2$ IR: 1745

^{13}C NMR: 185 (s), 155 (s), 135 (d), 130 (d), 128 (d), 65 (t), 28 (t), 19 (q)

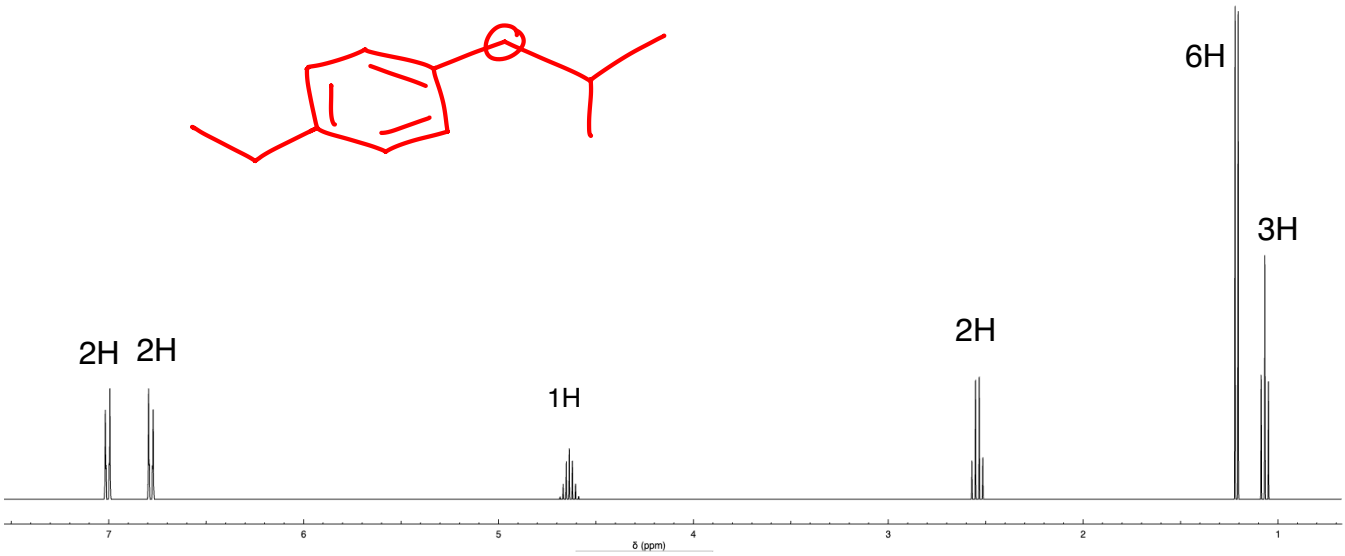


5. $C_5H_8O_2$ IR: 1720, 1725 2 ketones

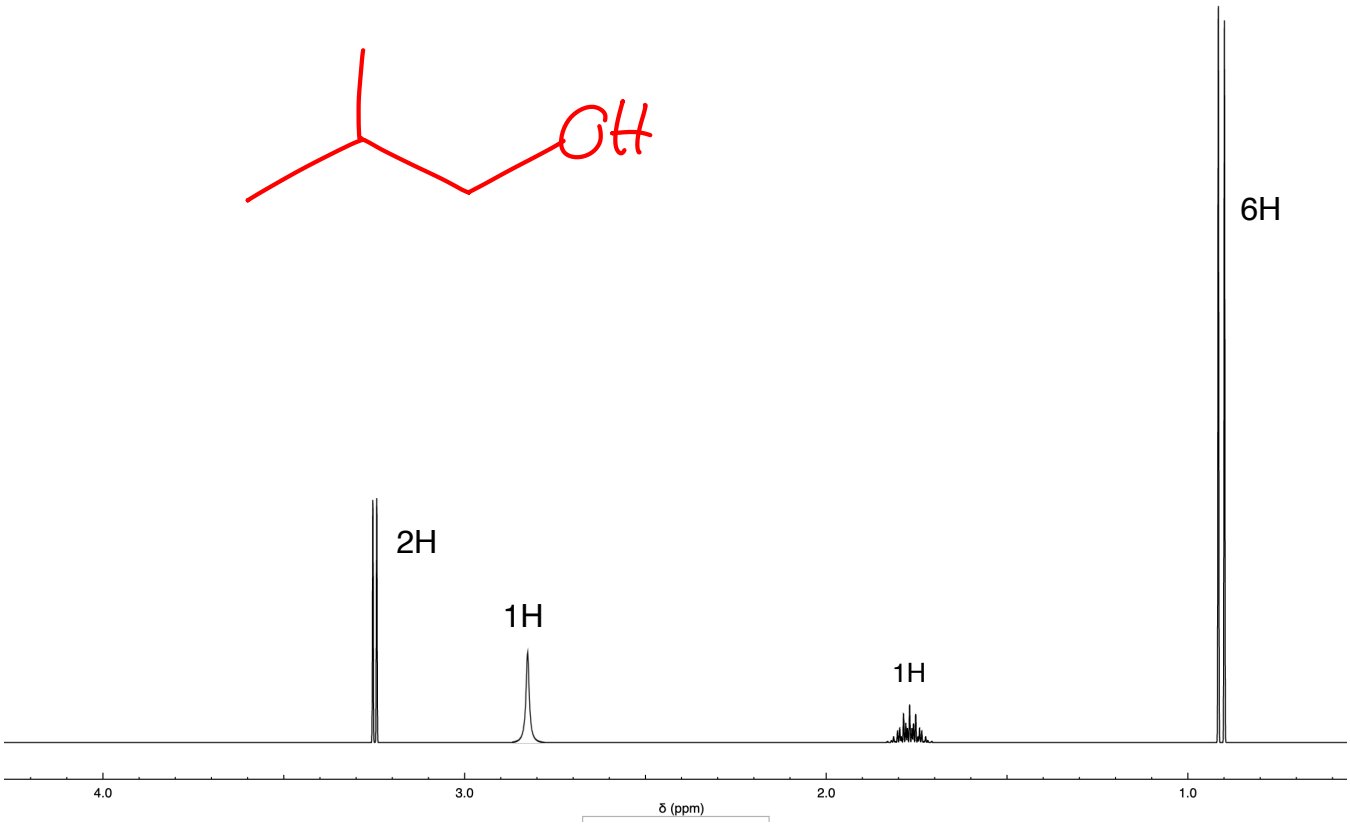


6. $C_4H_8Br_2$ IR: Nothing interesting

7. $C_{11}H_{16}O$ IR: nothing interesting
^{13}C: 158 (s), 141 (s), 128 (d), 114 (d), 65 (d), 29 (t), 22 (q, tall), 15 (q)



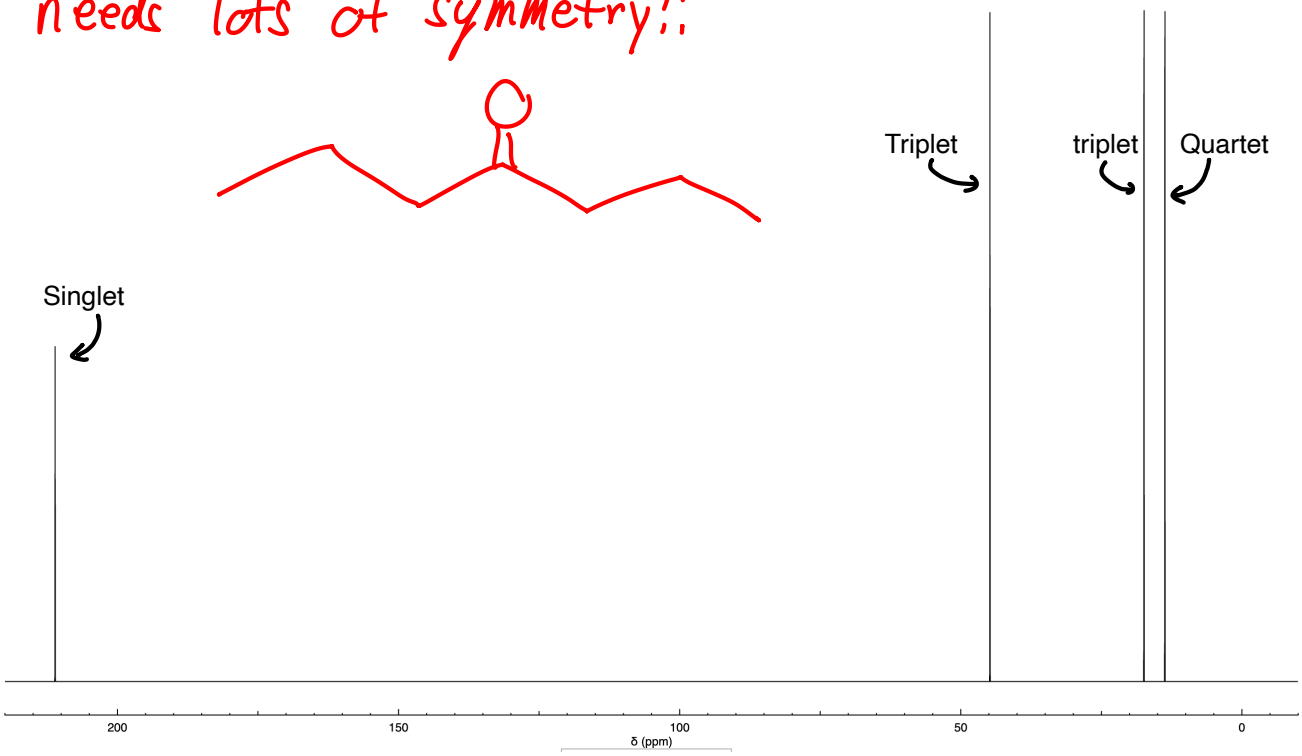
8. $C_4H_{10}O$ IR: 3300-3200



9. $C_7H_{14}O$ IR: 1710

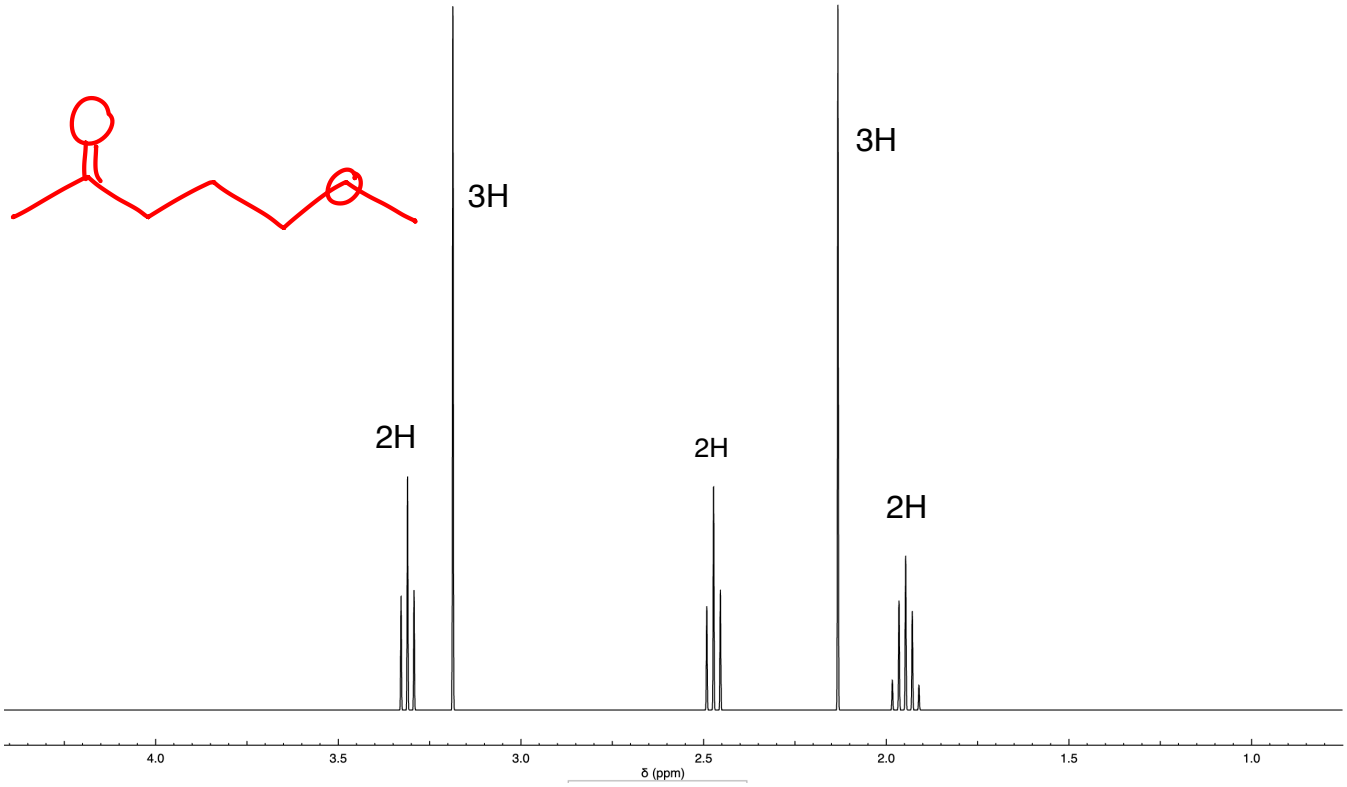
- The spectrum displayed is a "decoupled" 13-C NMR spectrum. (No splitting)
- But beside each coupled peak is a label that tells whether the carbon would be a singlet, doublet, triplet, or quartet **if** a "coupled" 13-C NMR had been obtained.

needs lots of symmetry!!



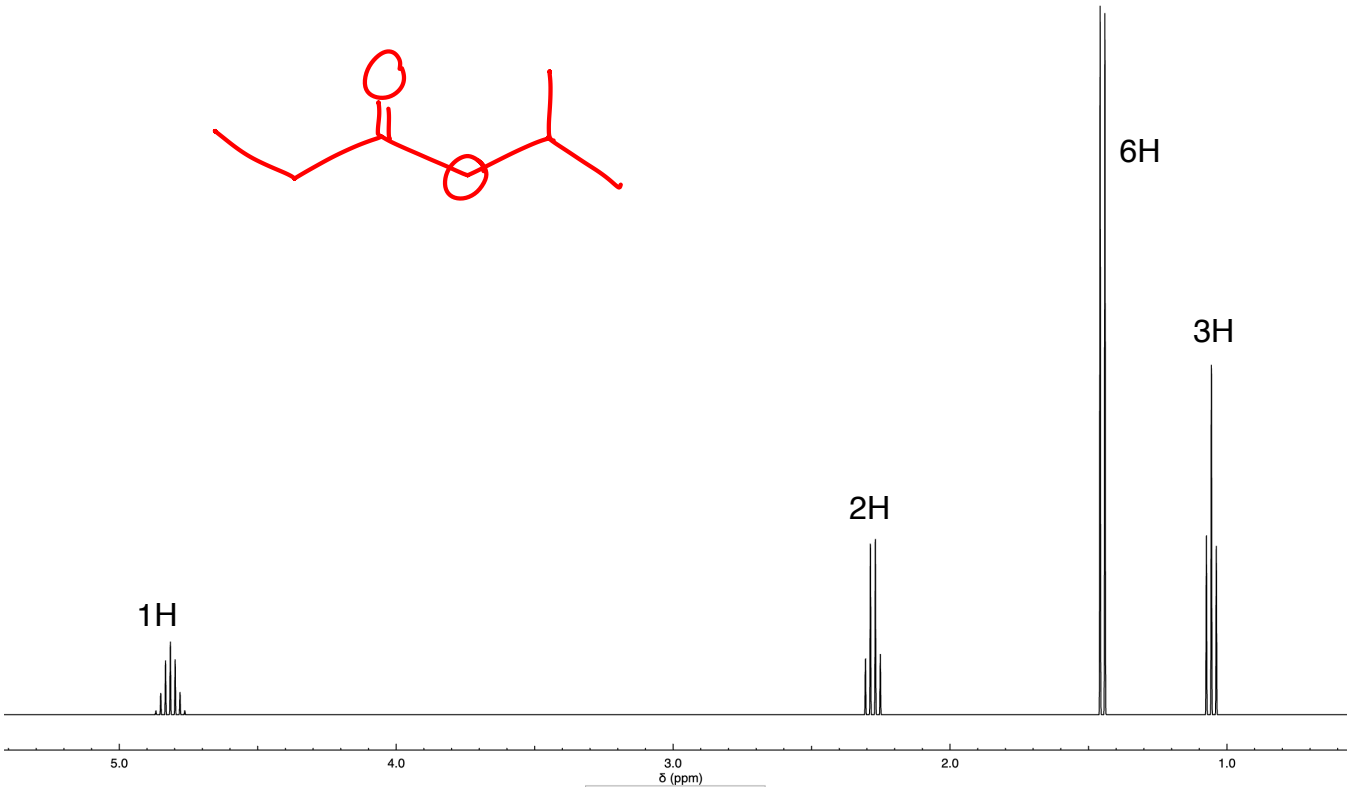
10. $C_6H_{12}O_2$ IR: 1710

13C-NMR: 210 (s), 75 (t), 65 (q), 40 (t), 30 (t), 20 (q), 20 (q)

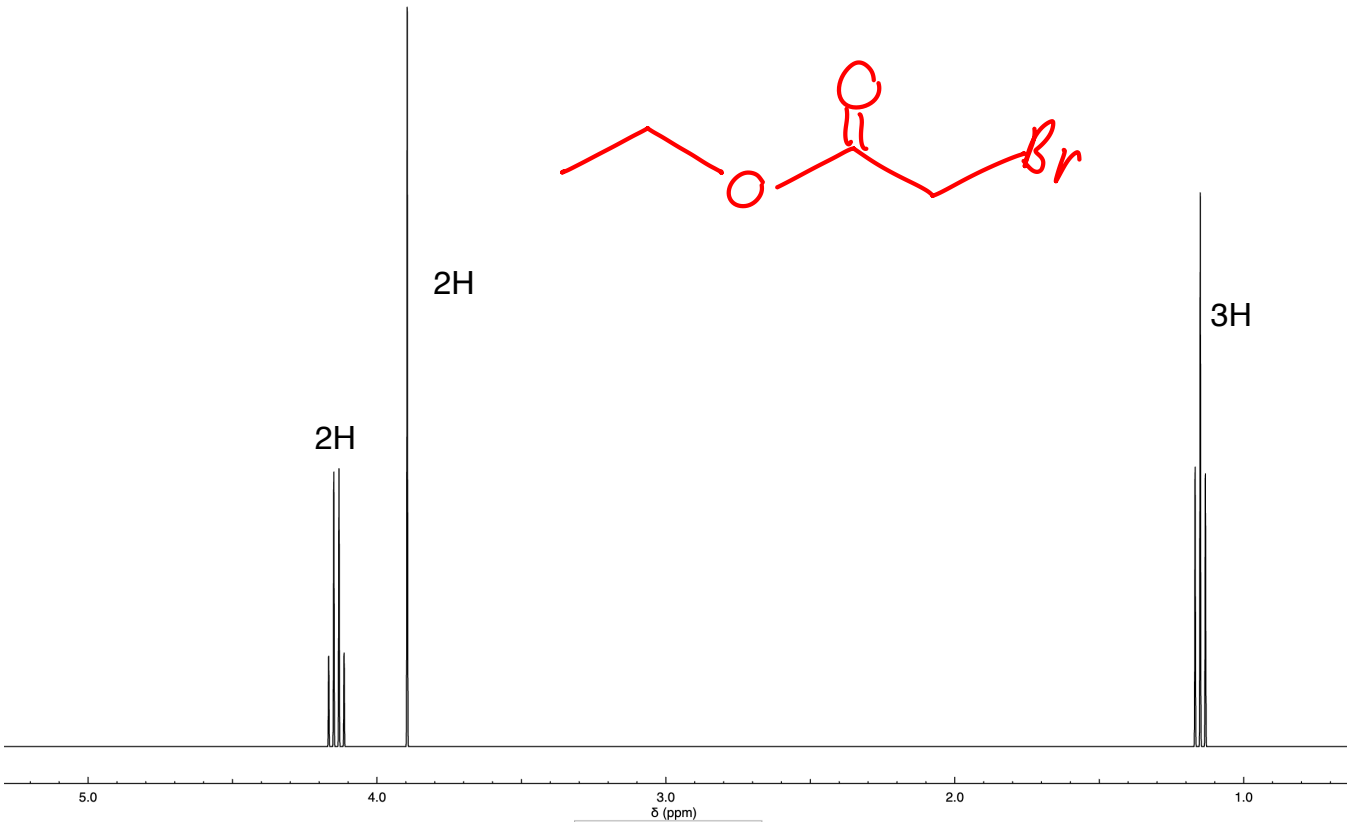


11. $C_6H_{12}O_2$ IR: 1745

13C-NMR: 185 (s), 78 (d), 42 (t), 30 (q), 20 (q)



11. $C_4H_7O_2Br$ IR: 1745



- 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.