

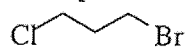
Ch. 12-13 NMR, IR

NOTE: This Version is Longer than the Real Test Will Be

1. Predict the ^1H NMR spectra for the following molecules. Include predicted:

- chemical shifts
- integration
- splitting pattern (singlet, doublet, triplet, quartet, etc., multiplet)

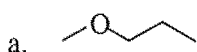
Example



3's, 2H, t

1's (or 2's), 2H, pentet (or multiplet)

3's, 2H, t



3's 3H s

3's 2H t

1's 2H m (or sextet)

1's 3H t

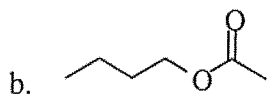
1's 3H t

1's 2H m (or sextet)

1's 2H p

3's 2H t

2's 3H s

2. Assign the dimethylbenzene isomer for which the ^{13}C NMR spectrum has:

a. 3 signals (q, s, d)



max symmetry

b. 4 signals (q, s, d, d)



c. 5 signals (q, s, d, d, d)



3. Match the circled proton or protons in the following compounds with the correct chemical shift.

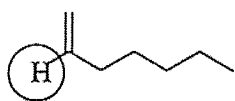
1.20

2.05

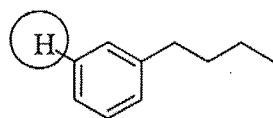
5.70

7.17

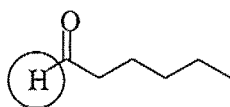
9.55



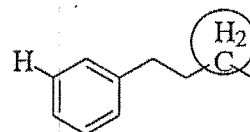
5.70



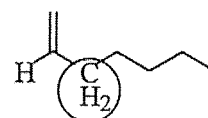
7.17



9.55



1.20



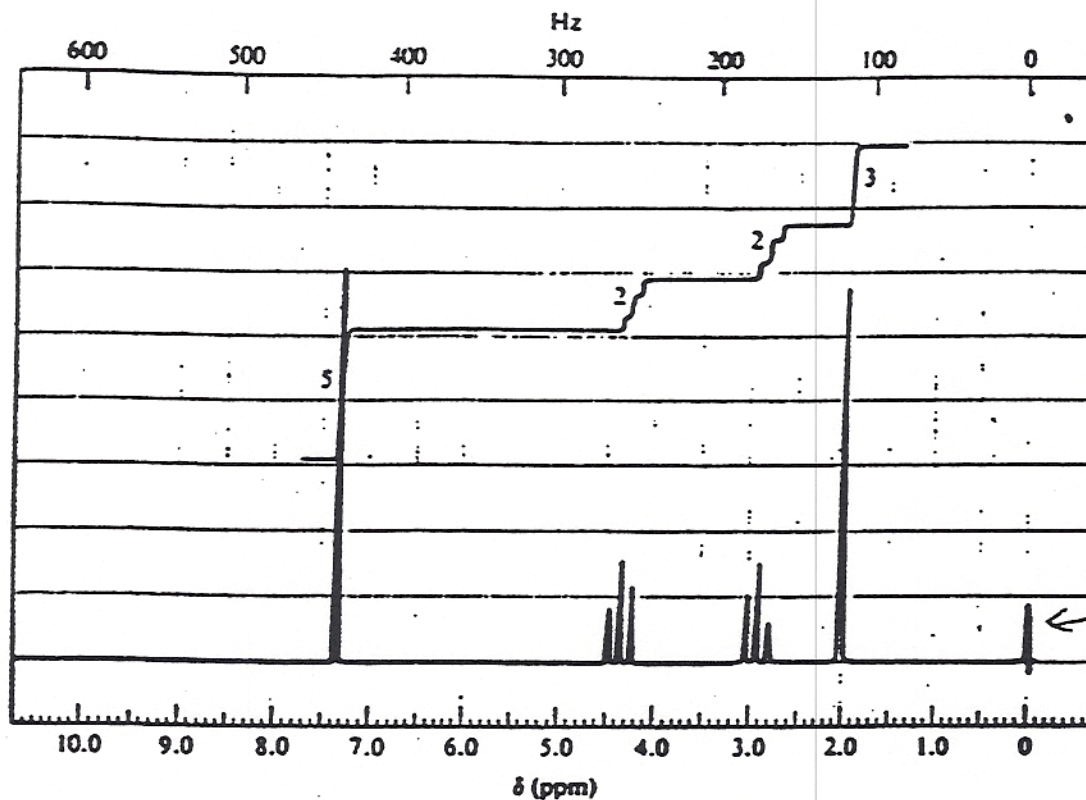
2.05

DRAW STRUCTURES FOR THE MOLECULES IN PROBLEMS 3-9



IR: 1740 (strong), 750 (strong), 700 (strong)

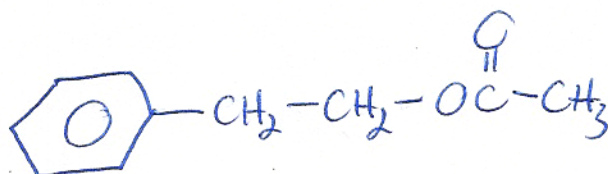
^{13}C NMR: 185 (s), 155 (s), 135 (d), 130 (d), 128 (d), 128 (d), ⁶⁵36 (t), 28 (t), 20 (q)



Note:
Signal at zero is reference signal, nothing in actual molecule.

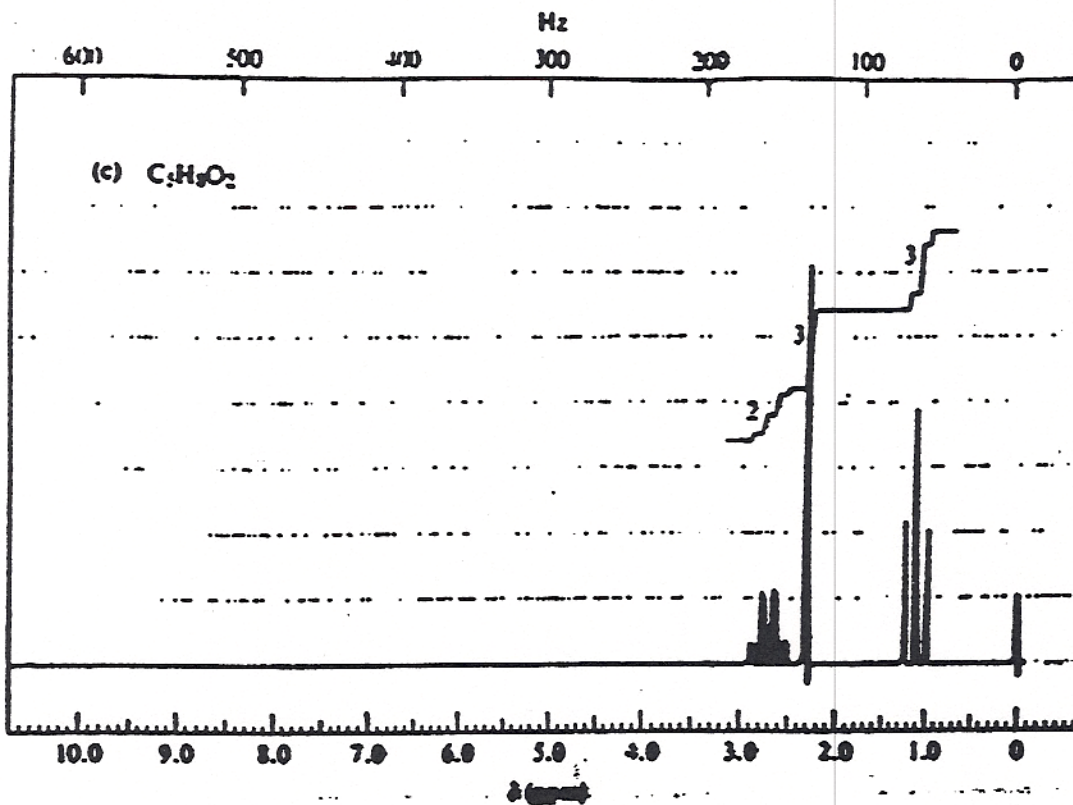
EU=5

IR \Rightarrow ester



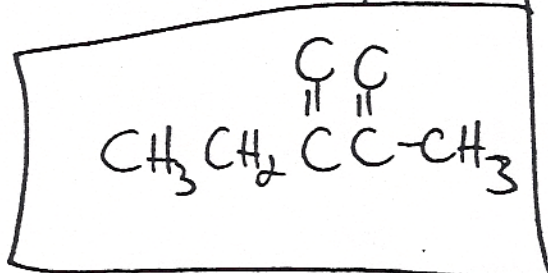


IR: 1720 (s), 1725 (s)



$EU=2$

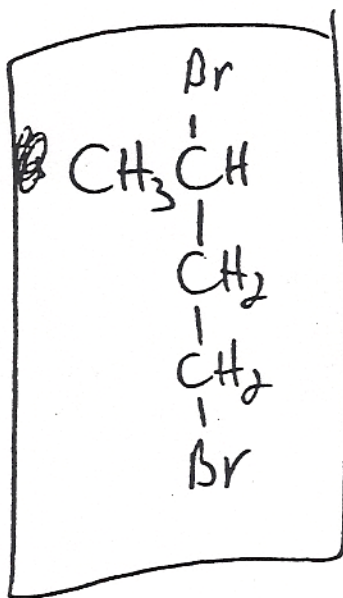
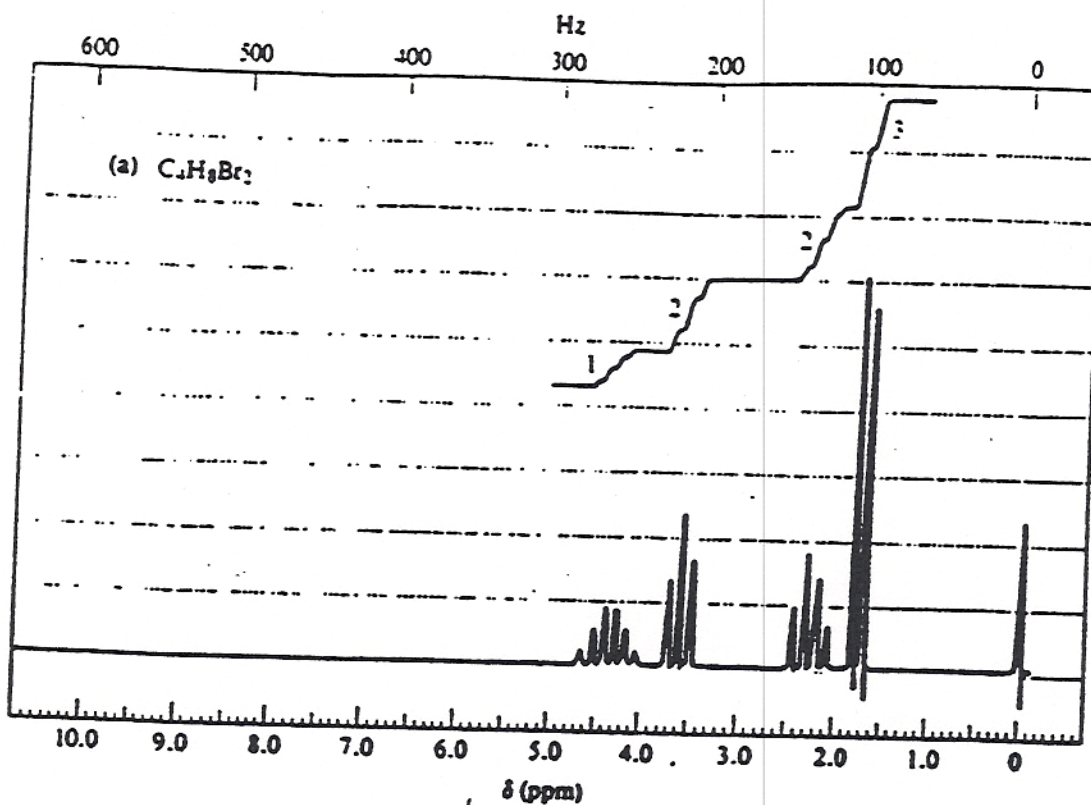
IR \Rightarrow 2 carbonyls



5. $C_4H_9Br_2$

IR: nothing interesting

^{13}C NMR: 45 (d), 37 (t), 24 (t), 18 (q)



6. $C_{11}H_{16}O$

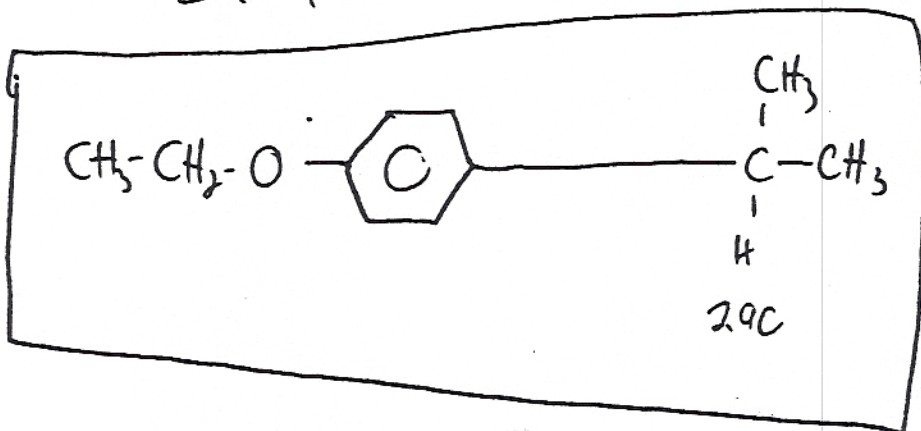
IR: 820 (strong)

^{13}C : 145 (s), 132 (s), 128 (d), 120 (d), 75 (t), 35 (d), 20 (q), 18 (q)

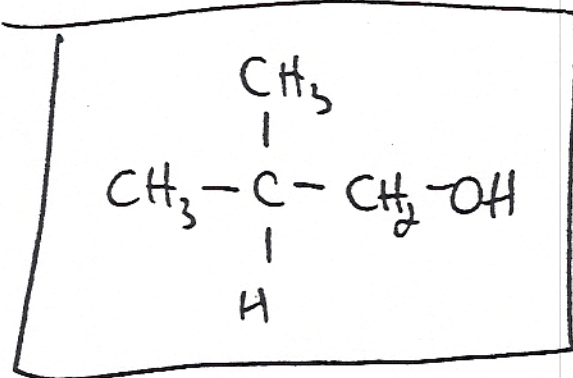
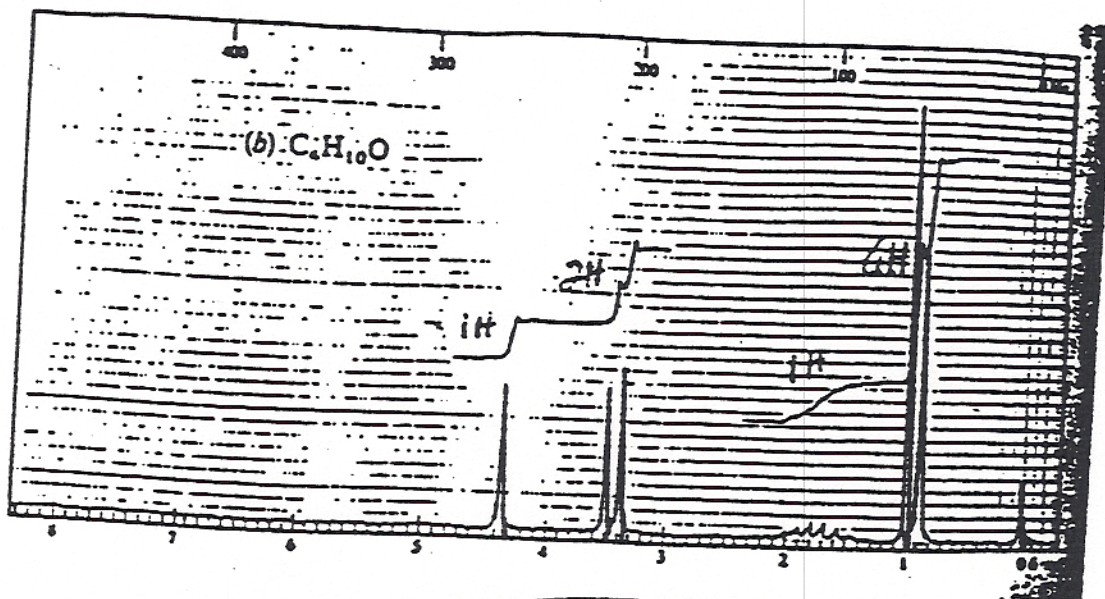
1H NMR: 1.25 (6H, d), 1.30 (3H, t), 2.90 (m, 1H), 4.15 (2H, q), 6.66 (2H, d), ~~6.97 (2H, d)~~

EU = 4

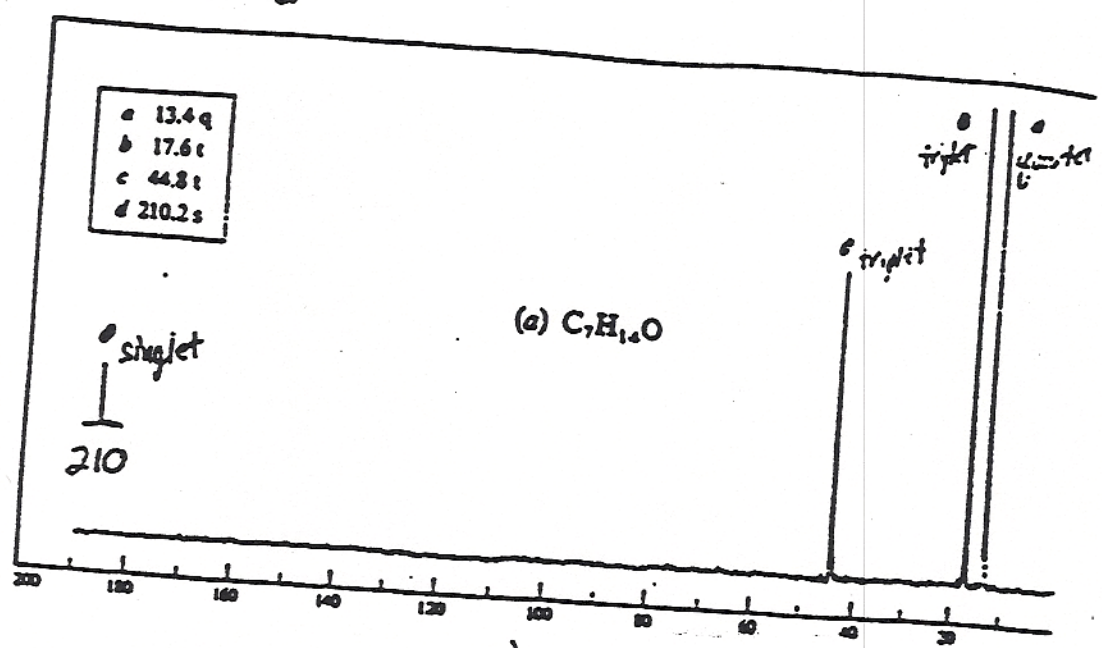
~~6.97~~ disabled



$C_4H_{10}O$



$C_7H_{14}O$
IR: 1710 (strong)



need symmetry!!

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13. Show the structures for the following molecule, based on the spectroscopic information provided. (10 points)

$C_6H_{12}O_2$

IR: 1710; strong

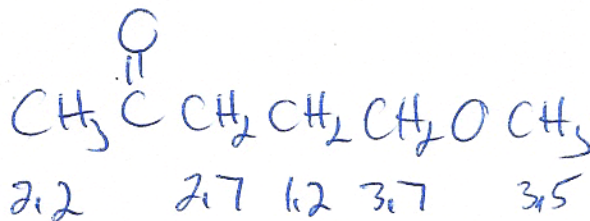
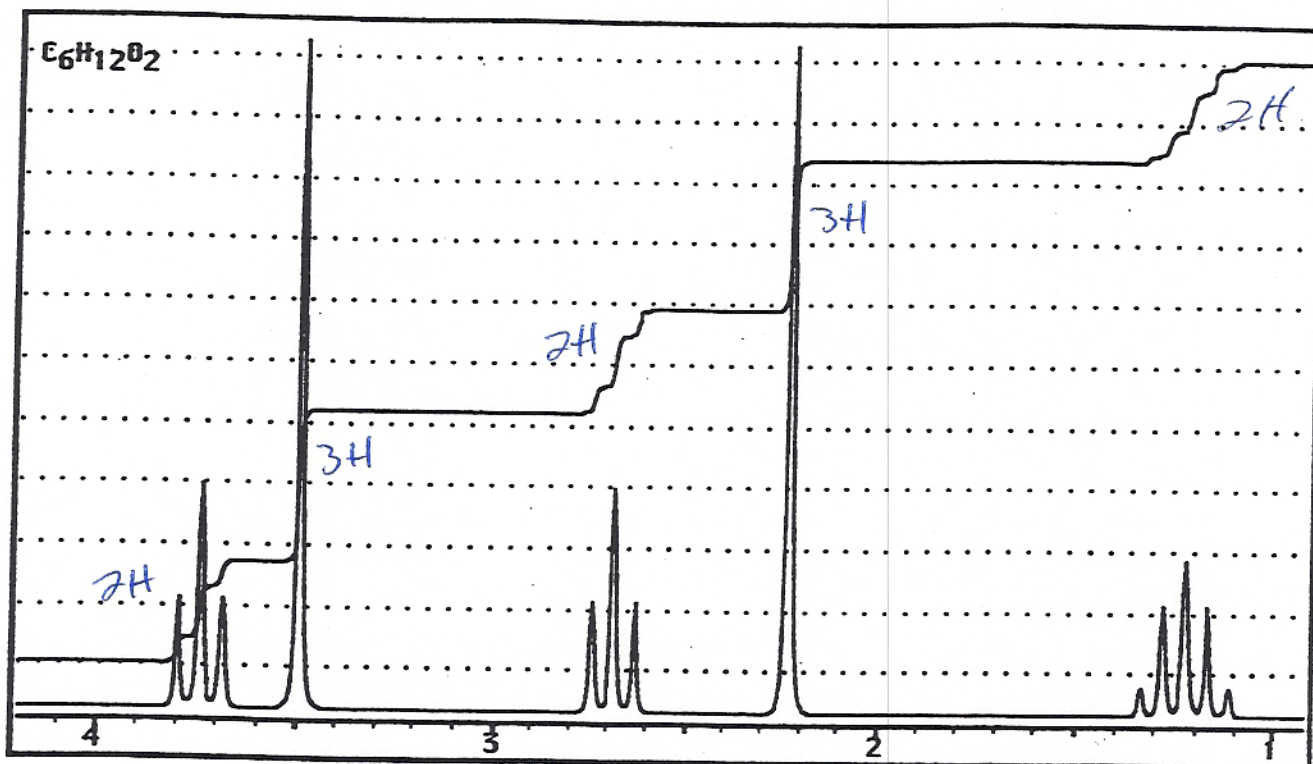
^{13}C NMR: 200 (s), 75 (t), 65 (q), 40 (t), 30 (t), 20 (q)

$EU=1$

$C=O$

no O-H

not ester



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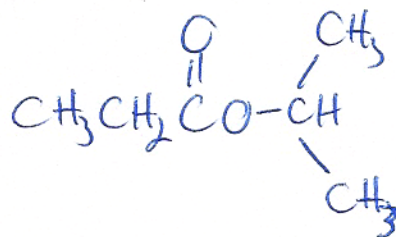
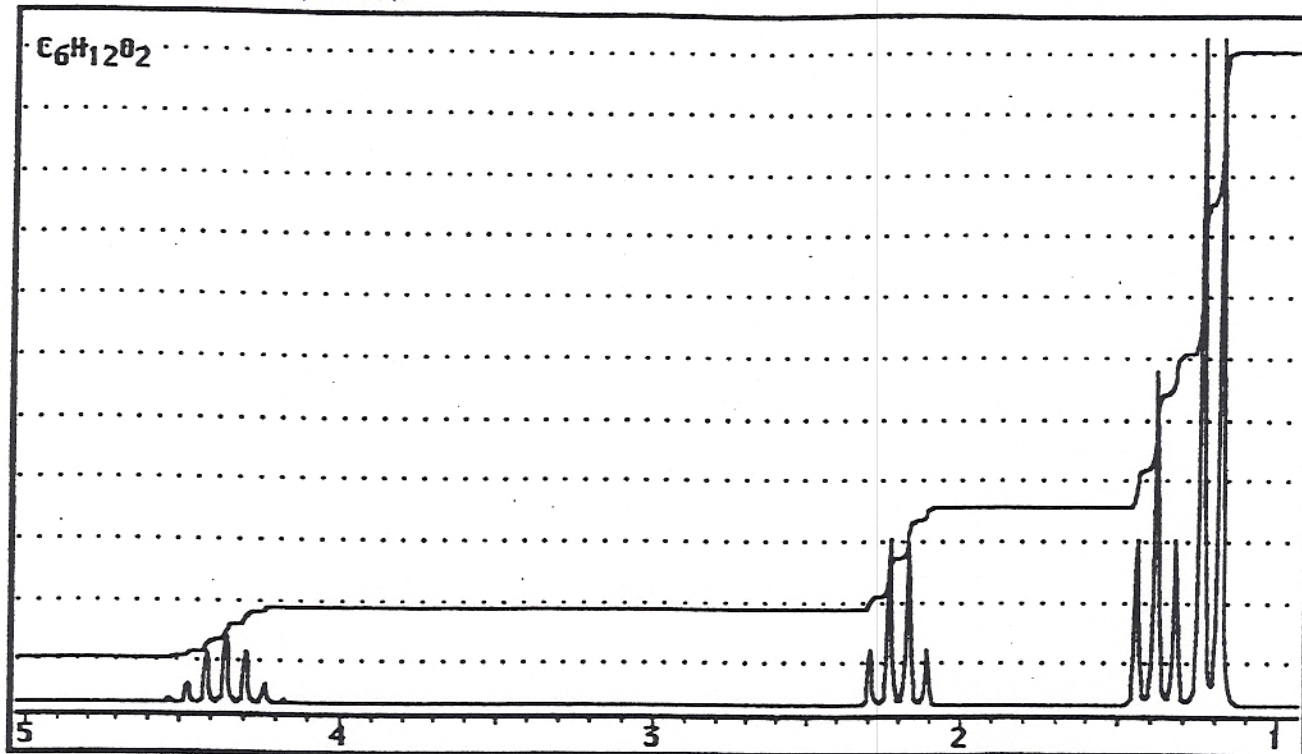
16. Show the structures for the following molecule, based on the spectroscopic information provided. (10 points)

$C_6H_{12}O_2$ IR: 1745, strong

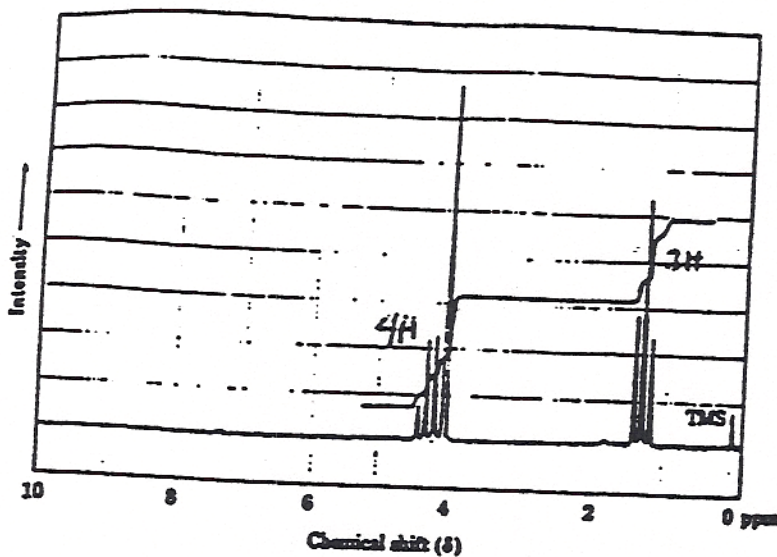
^{13}C NMR: 20 (q), 30 (q), 48 (t), 78 (d), 185 (s)

EU=1

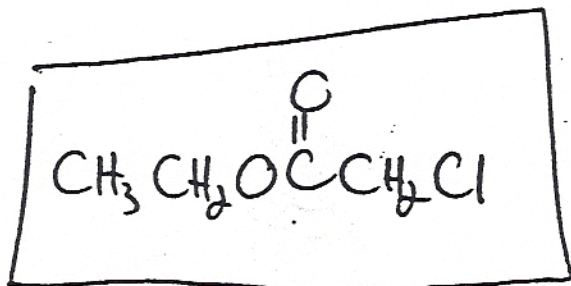
$C=O$,
no OH
1745 \rightarrow ester



9, C₄H₇O₂Cl
IR: 1740



EU = 1
IR ⇒ ester



2011