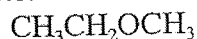


## NMR, IR

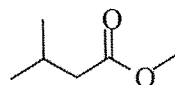
## 1. Predict the:

- $^1\text{H}$  NMR spectrum [include approximate chemical shifts (1's, 2's, 3's, 4's, 5's, etc.), integration, and splitting]
- $^{13}\text{C}$  NMR spectrum [include approximate chemical shifts (0-50, 50-100, 100-150, or 150-220) and splitting]
- identify any distinctive signals in the IR spectrum

Example:



$^1\text{H}$ NMR			$^{13}\text{C}$ NMR	IR
1's	3H	t	0-50, q	none
3's	2H	q	50-100, t	
3's	3H	s	50-100, q	



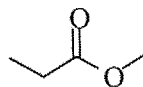
$^1\text{H}$ NMR			$^{13}\text{C}$ NMR	IR
1's	6H	d	0-50 q	1700's
1's	1H	m	0-50 d	(~1745)
2's	2H	d	0-50 +	
3's	3H	s	220-150 s	
			50-100 q	

## 2. For the following molecule,

- Write how many "types" of H's there would be in the  $^1\text{H}$  NMR spectrum (these are H's which might coincidentally overlap, but can't be assumed to be chemical shift equivalent)
- Write how many different  $^{13}\text{C}$  NMR absorptions you would expect, and
- Write what the  $^{13}\text{C}$  NMR splitting would be, i.e. singlet, doublet, triplet, or quartet for the  $^{13}\text{C}$  NMR absorptions.

Number of Nonequivalent H's in H-NMR	Number of $^{13}\text{C}$ Absorptions in $^{13}\text{C}$ NMR	Expected Splittings in $^{13}\text{C}$ NMR
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Example:



3

4

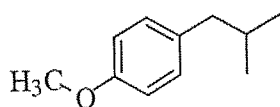
q, t, s, q

Number of Nonequivalent H's in H-NMR	Number of $^{13}\text{C}$ Absorptions in $^{13}\text{C}$ NMR	Expected Splittings in $^{13}\text{C}$ NMR
--------------------------------------	--	--

6

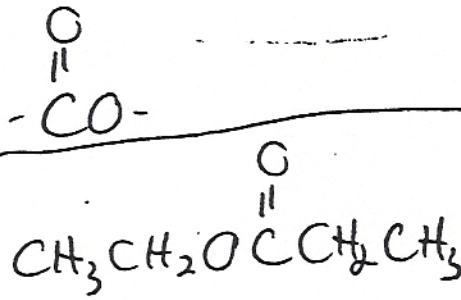
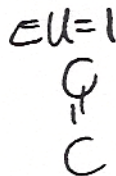
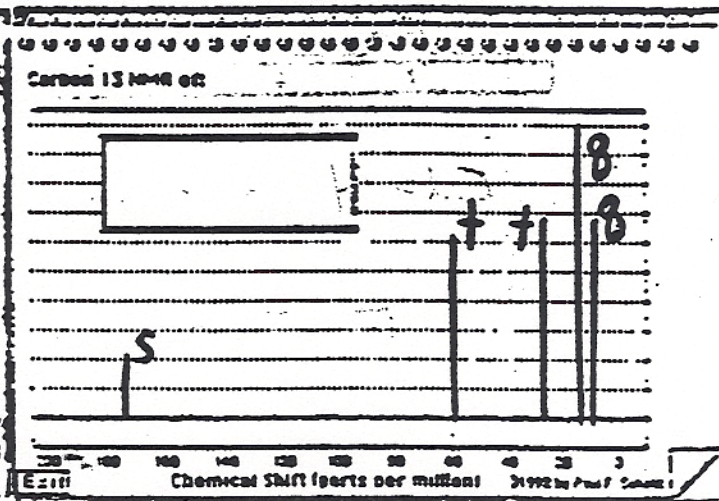
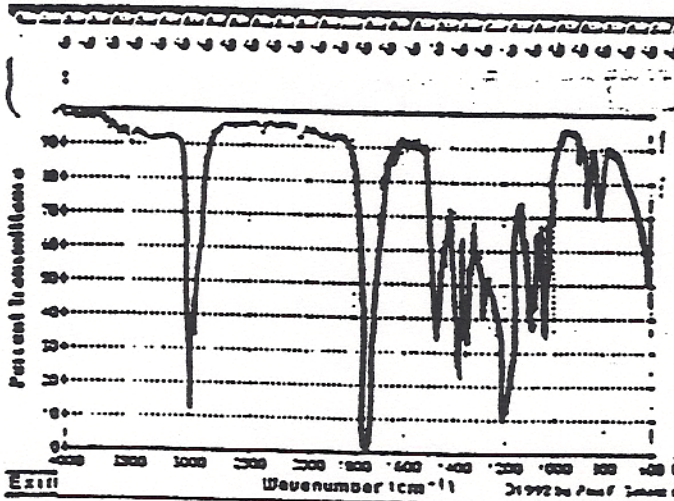
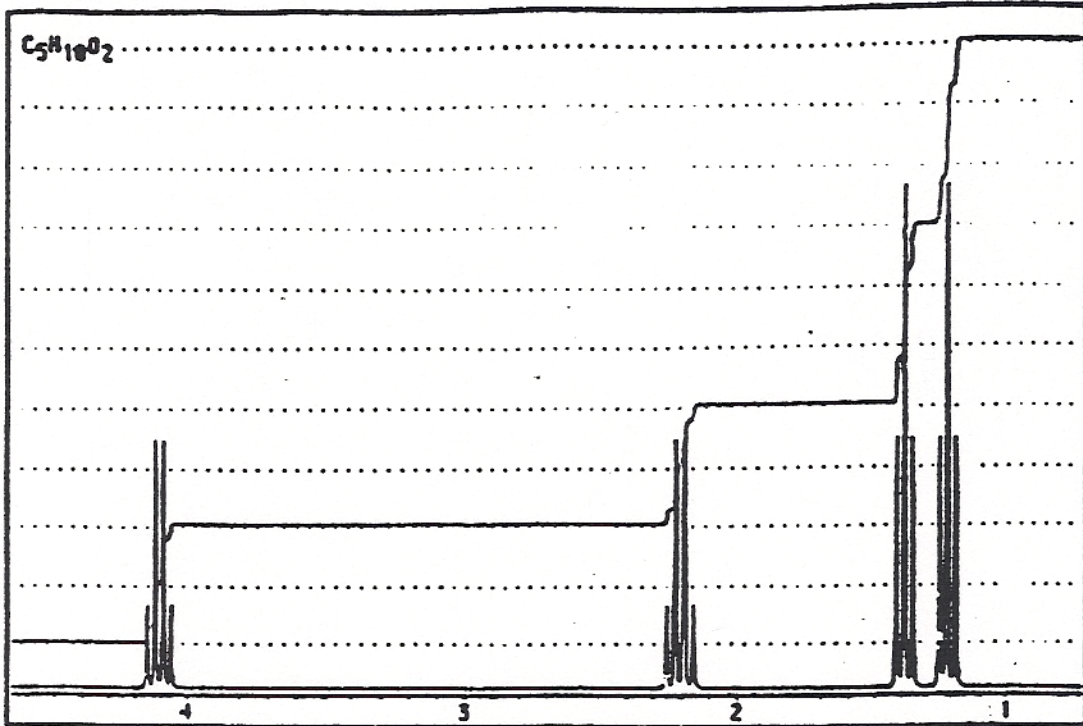
8

q, s, d, d  
s + d, q



Provide Structures Based on the Following Spectroscopic Data (8 points each)

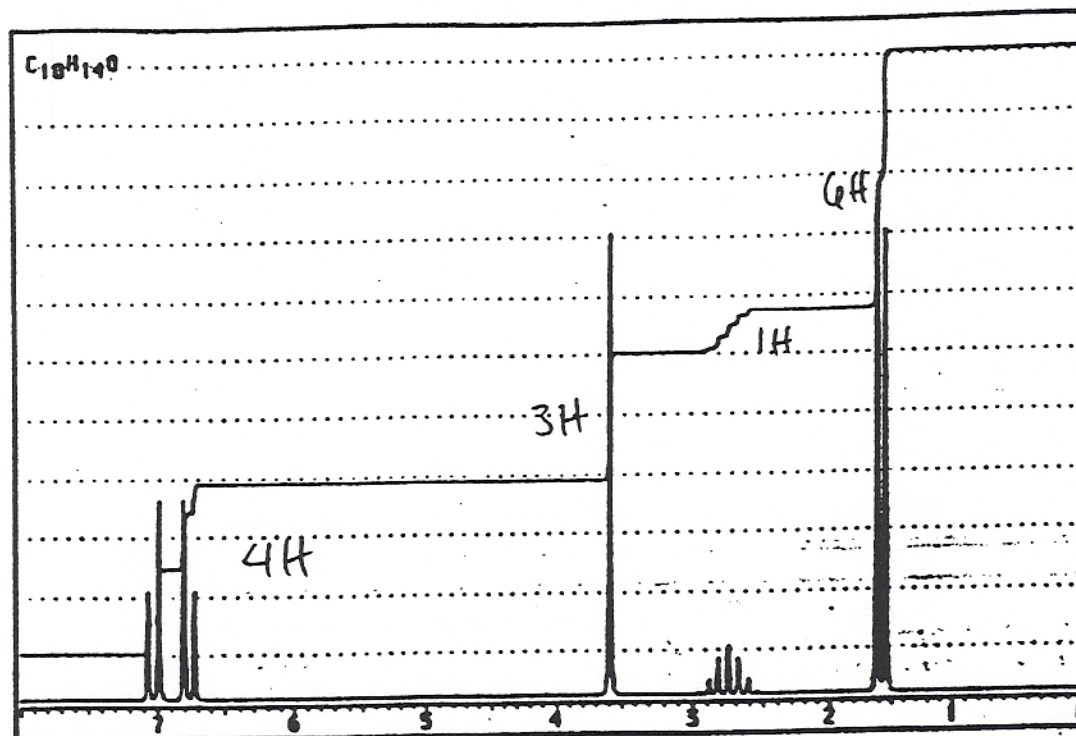
4.  $C_5H_{10}O_2$



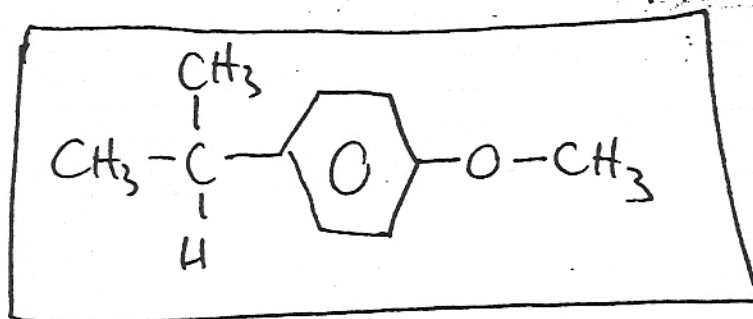
5. C<sub>10</sub>H<sub>14</sub>O

<sup>13</sup>C NMR:

148	s	135	d	75	q	50	d
122	s	128	d			22	q



EU = 4    disubbed    para, from <sup>13</sup>C

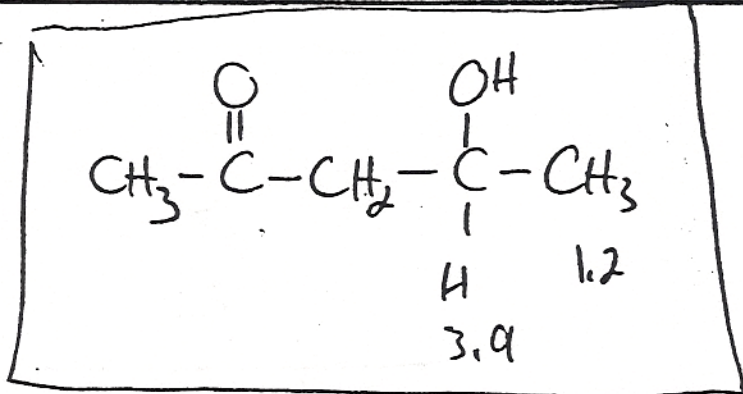
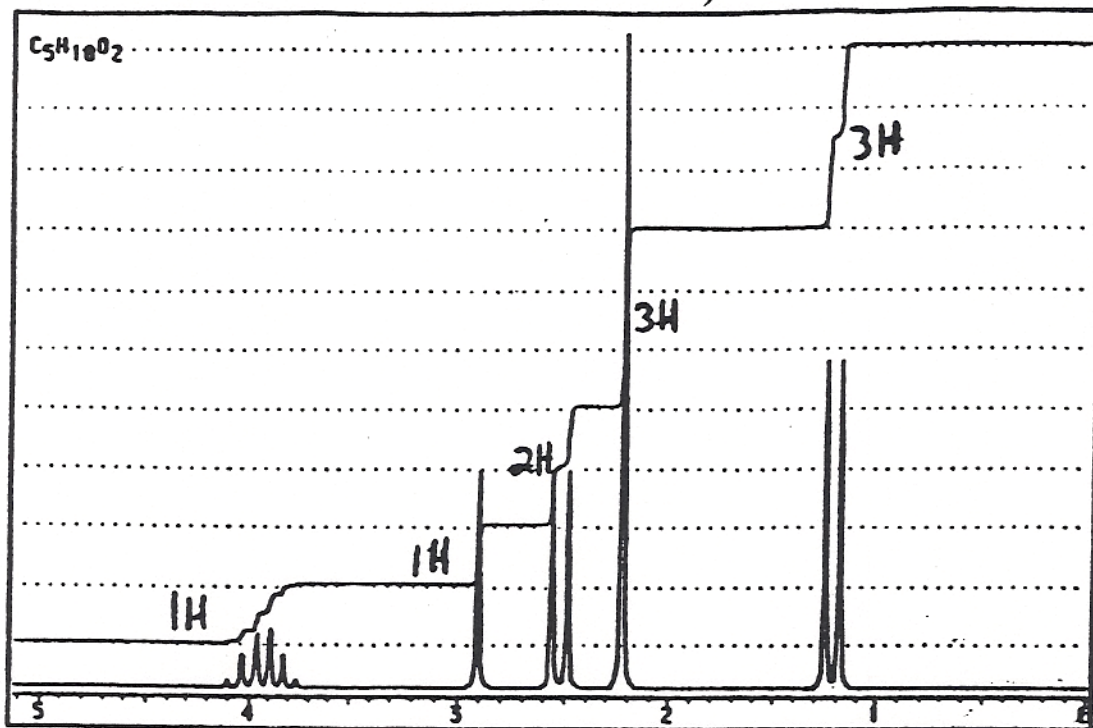


6.  $C_5H_{10}O_2$

IR: 1710 (strong), 3300-3500 (broad, strong)

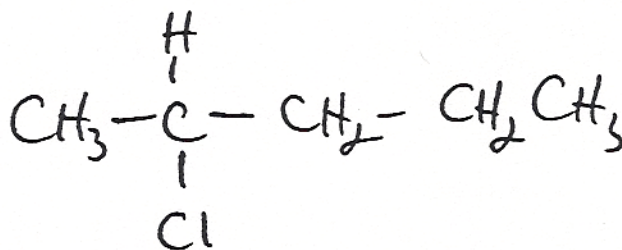
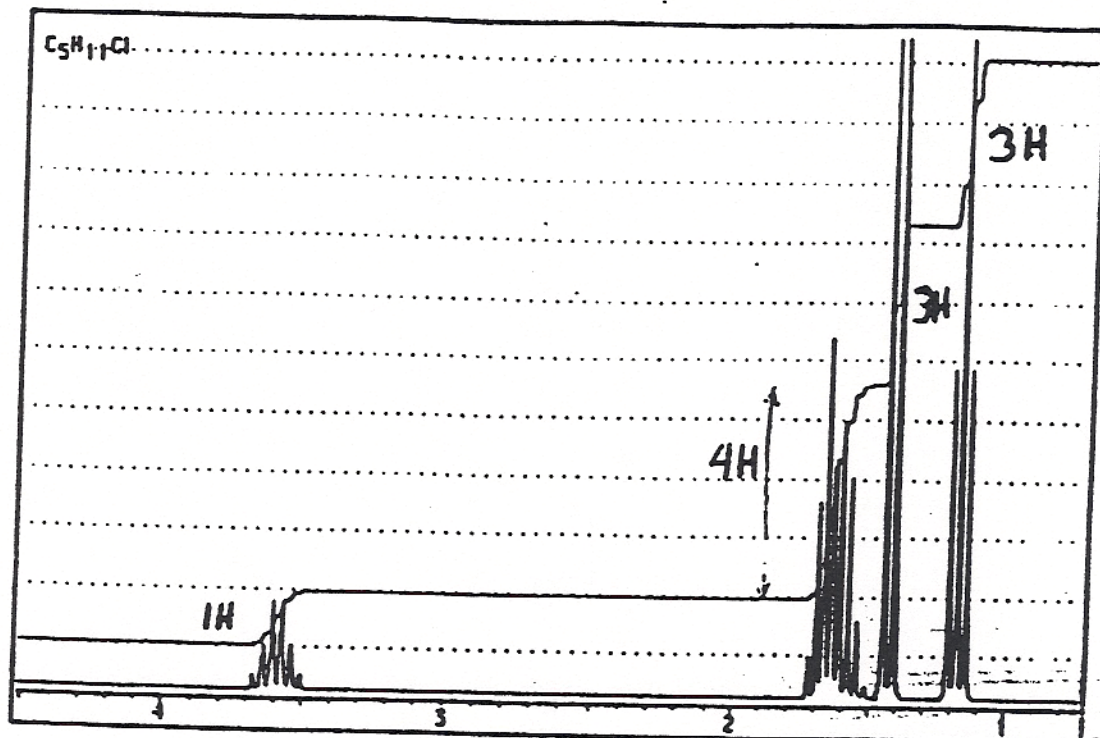
↳ C=O

↳ OH (not acid)

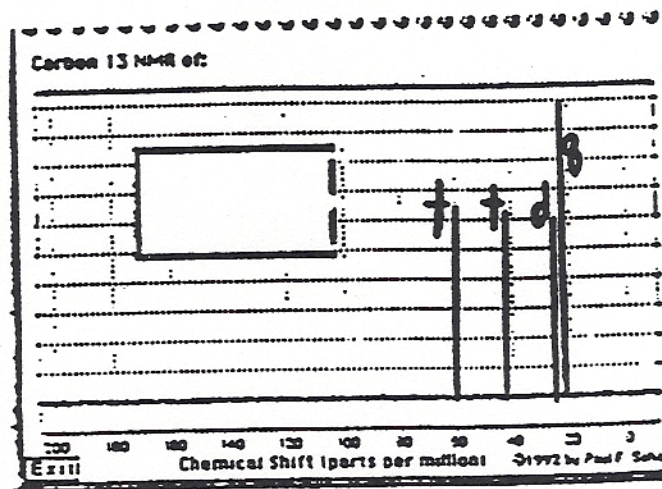
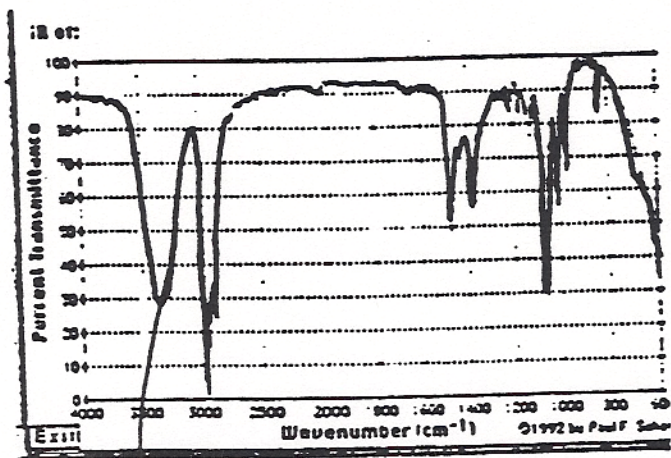
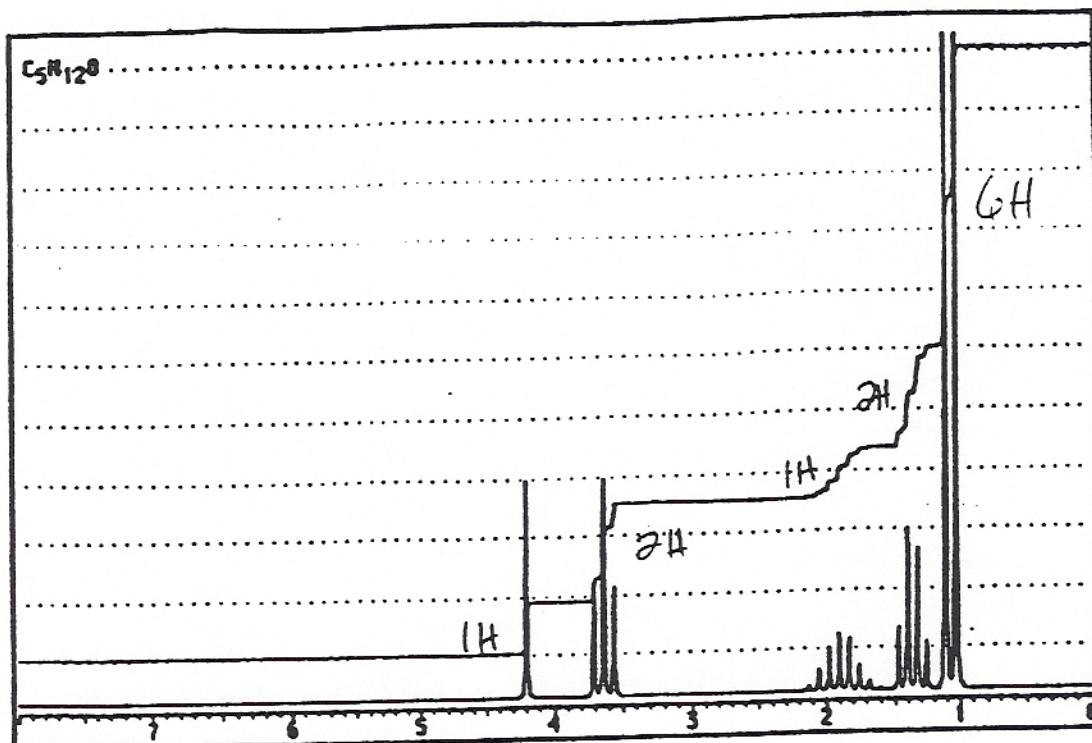


7.  $C_5H_{11}Cl$

$^{13}C$  NMR: 60 (d), 40 (t), 37 (t), 33 (q), 20 (q) no symmetry

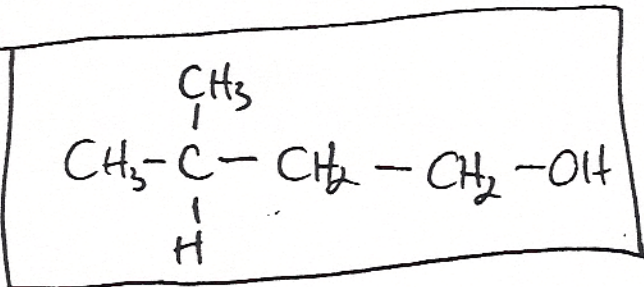


8. C<sub>5</sub>H<sub>12</sub>O



OH

symmetry



no other  
CH<sub>3</sub>'s, 7  
so other  
end must be OH

9. C<sub>4</sub>H<sub>8</sub>O<sub>2</sub> EU=1  
triplet, 1.02, 3H  
sextet, 1.43, 2H  
triplet, 2.35, 2H  
singlet, 10.95, 1H

IR 1715 cm<sup>-1</sup> and broad 2500-3000

