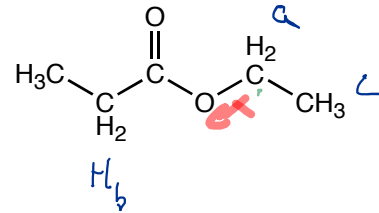


# of peaks = # of chemically different H's  
*sometimes different H's overlap*

H<sub>b</sub> are 3 bonds away from 2 O atoms, also deshielded, but not as much



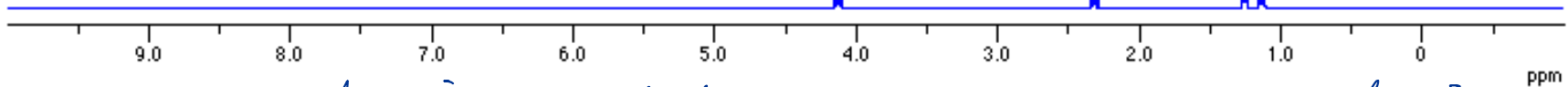
H<sub>c</sub> H<sub>a</sub> are 2 bonds from O atom + 4 bonds away from 2<sup>nd</sup> O

H<sub>2</sub> 3 bonds away from 1 O atom weakly deshielded

H<sub>d</sub> only slightly deshielded because they are 4 bonds from O atom

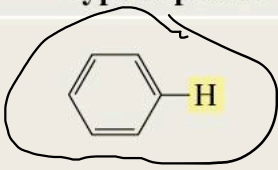
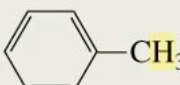
H<sub>a</sub>  
 farthest left = most deshielded

deshielded

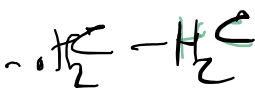


Chemical shift = position of peak in spectrum

Table 14.1 Approximate Values of Chemical Shifts for  $^1\text{H}$  NMR<sup>a</sup>

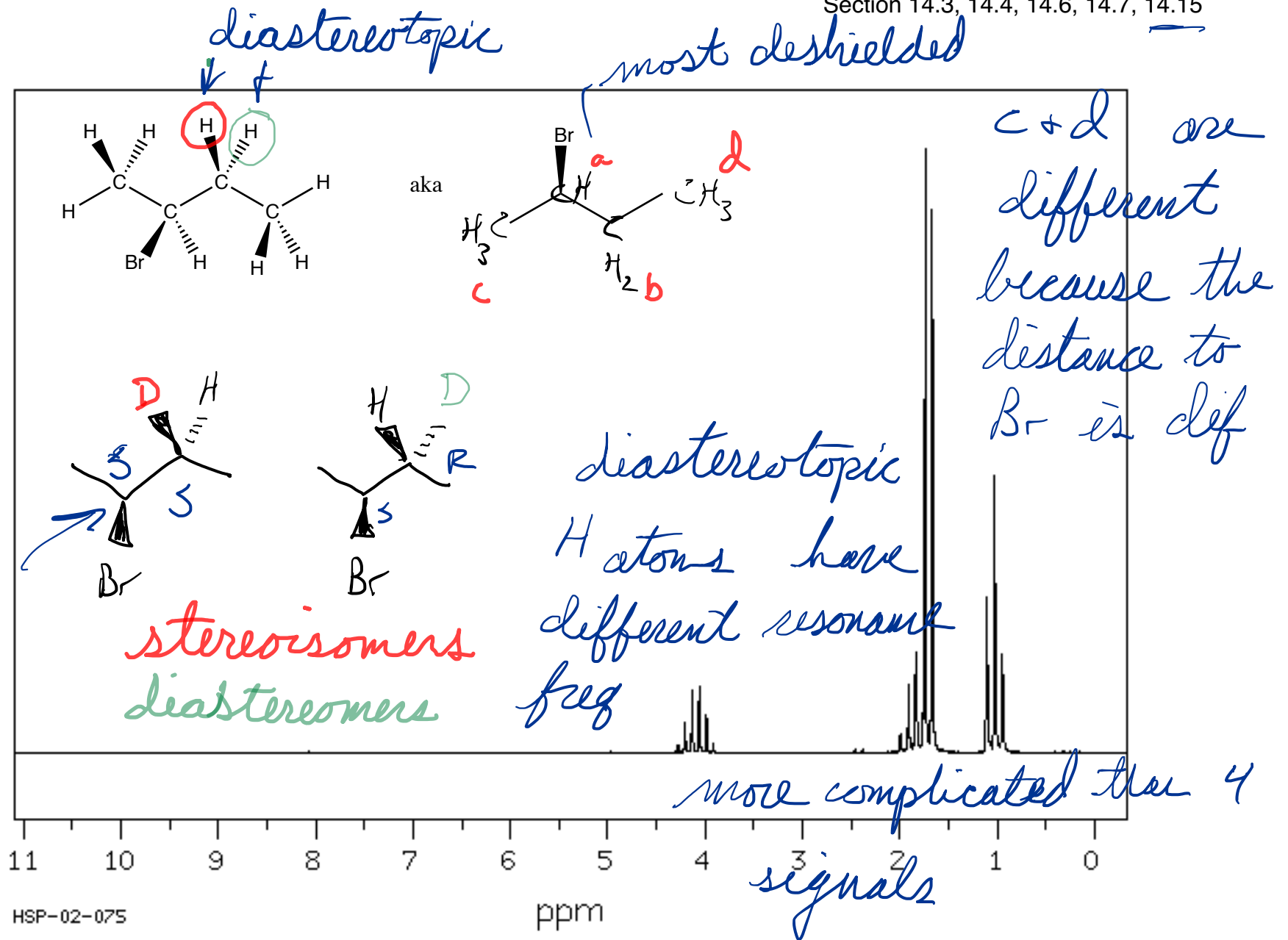
Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(\text{CH}_3)_4\text{Si}$	0		6.5–8
$-\text{CH}_3$	0.9	$-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$	9.0–10
$-\text{CH}_2-$	1.3	$\text{I}-\text{C}-\text{H}$	2.5–4
$-\overset{ }{\text{C}}\text{H}-$	1.4	$\text{Br}-\text{C}-\text{H}$	2.5–4
$-\overset{ }{\text{C}}=\overset{ }{\text{C}}-\text{CH}_3$	1.7	$\text{Cl}-\text{C}-\text{H}$	3–4
$-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3$	2.1	$\text{F}-\text{C}-\text{H}$	4–4.5
	2.3	$\text{RNH}_2$	Variable, 1.5–4
$-\text{C}\equiv\text{C}-\text{H}$	2.4	$\text{ROH}$	Variable, 2–5
$\text{R}-\text{O}-\text{CH}_3$	3.3	$\text{ArOH}$	Variable, 4–7
$\text{R}-\overset{\text{R}}{\underset{ }{\text{C}}}=\text{CH}_2$	4.7	$-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	Variable, 10–12
$\text{R}-\overset{\text{R}}{\underset{ }{\text{C}}}=\overset{\text{R}}{\underset{ }{\text{C}}}-\text{H}$	5.3	$-\overset{\text{O}}{\parallel}{\text{C}}-\text{NH}_2$	Variable, 5–8

<sup>a</sup>The values are approximate because they are affected by neighboring substituents.



*H bonding affects e<sup>-</sup> density*

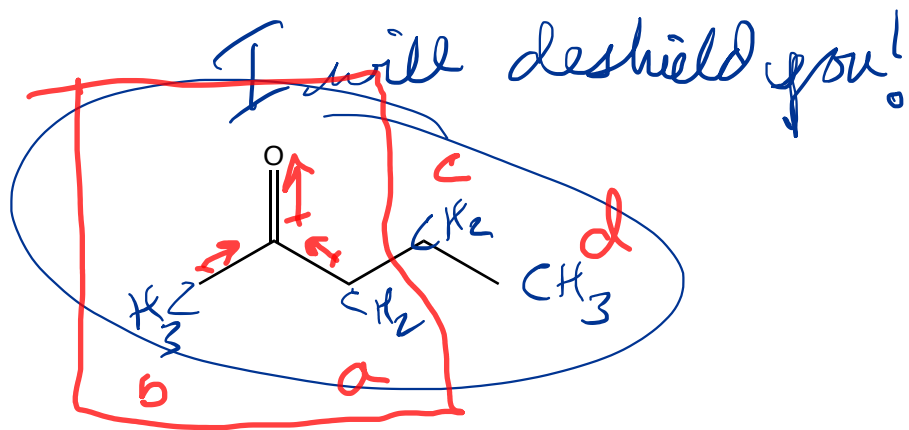
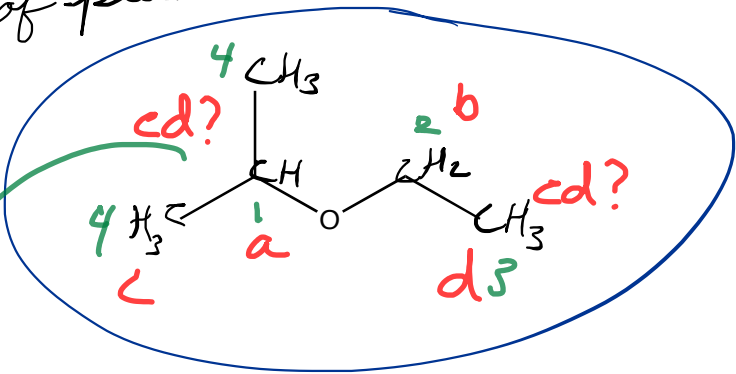
*tend to be broad*



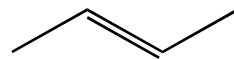
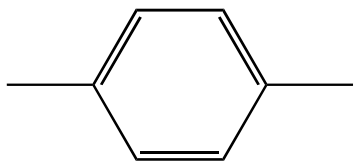
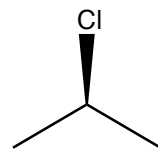
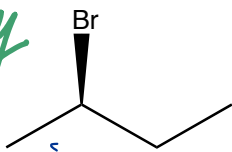
<https://sdfs.db.aist.go.jp/sdfs/cgi-bin/landingpage?sdfsno=500>

Check  $\text{CH}_2$ 's for diastereotopicity

# of peaks

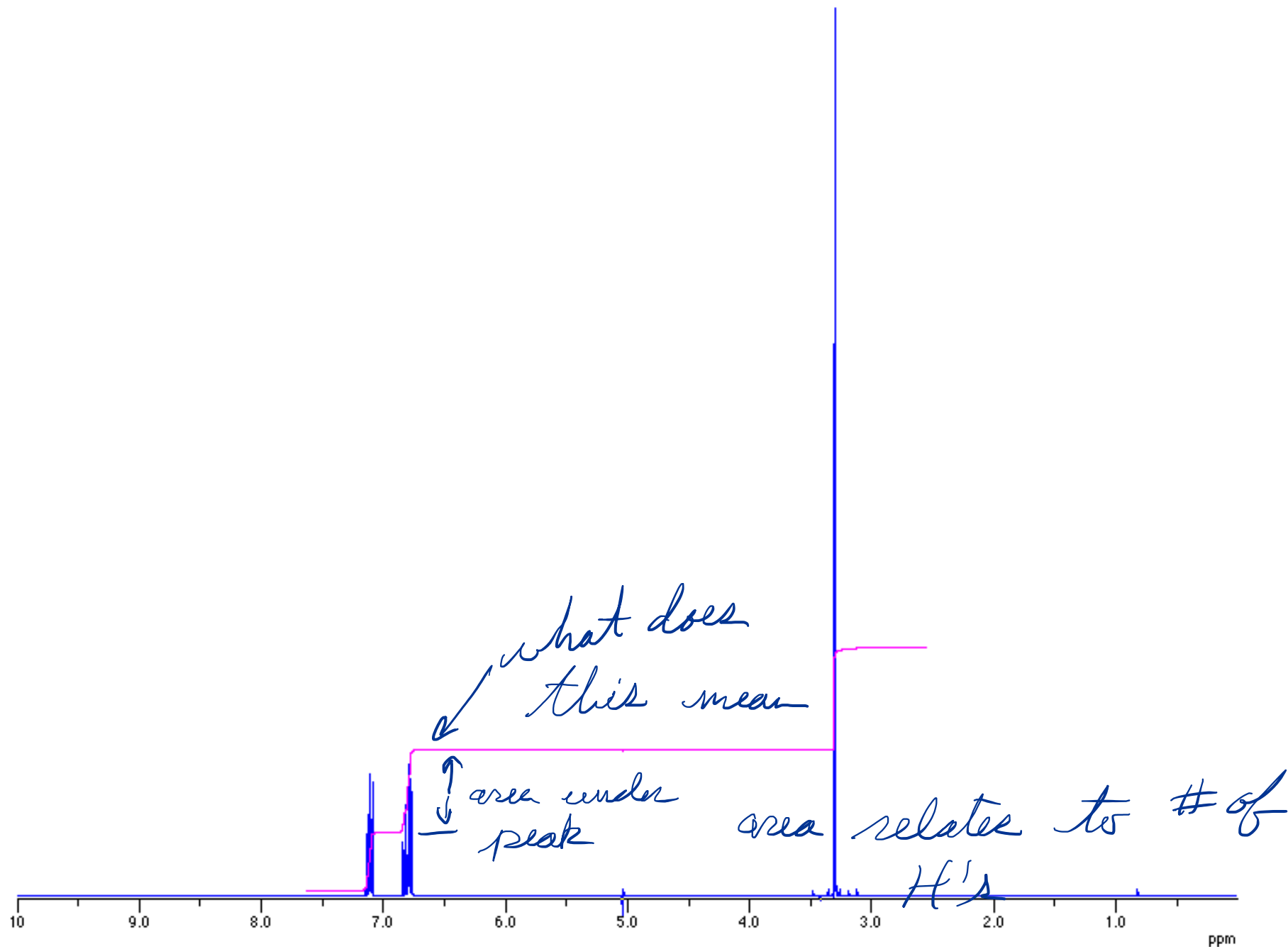


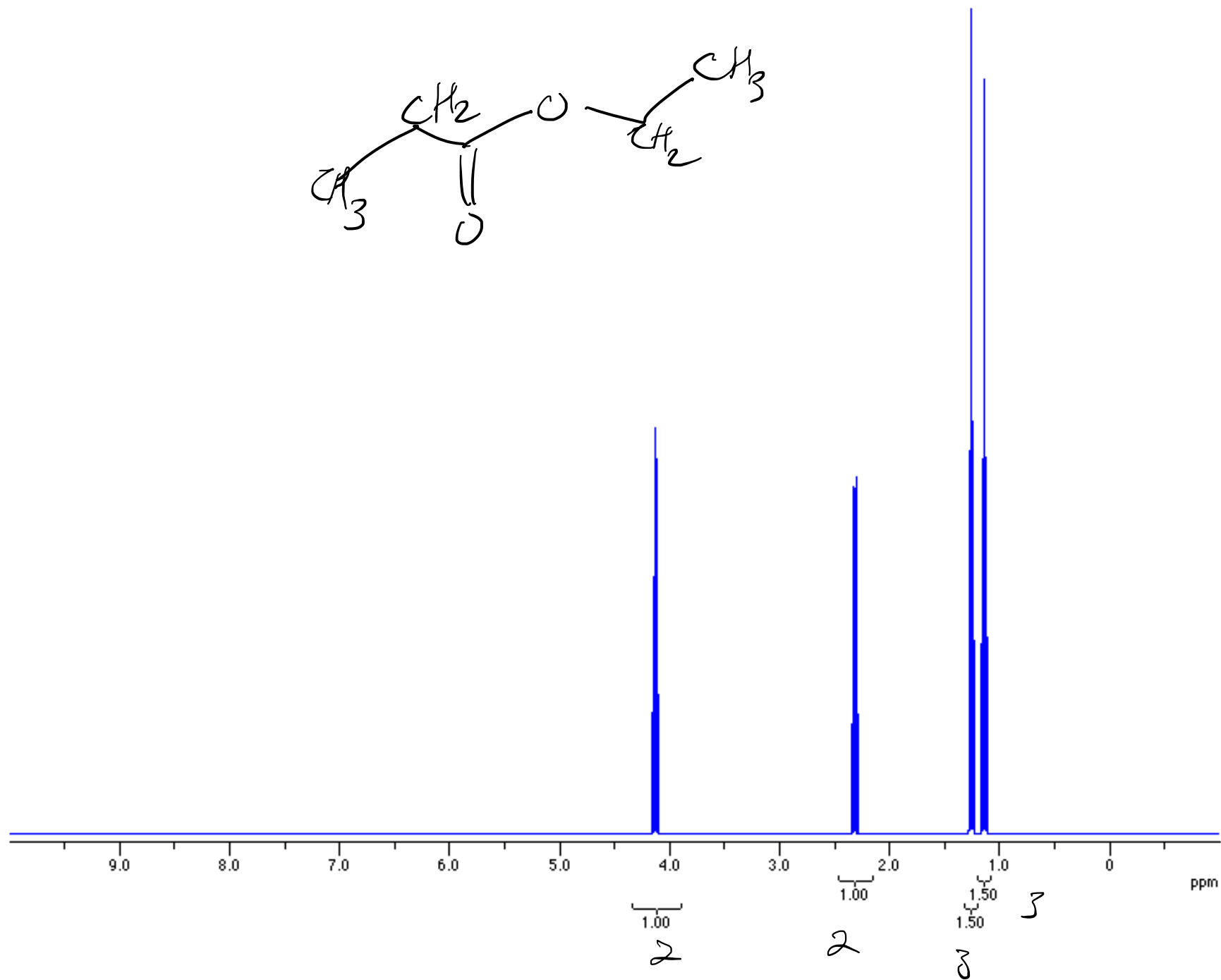
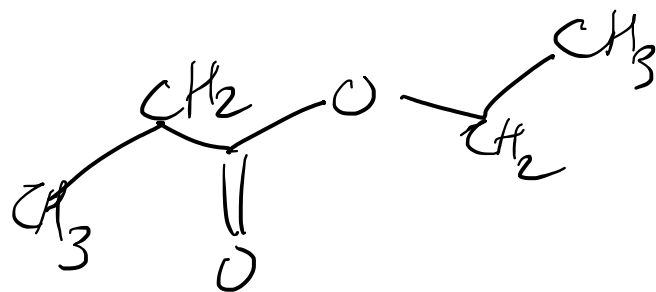
local symmetry



Number of different types of H atoms

Chemical environments of the H atoms





Number of different types of H atoms

# of signals

Chemical environments of the H atoms

to the left... near  $e^-$  withdrawal

How many of each type of H atom

From the integration



# Integration

1 find lowest whole number ratio

2 count up number of H's and compare to formula

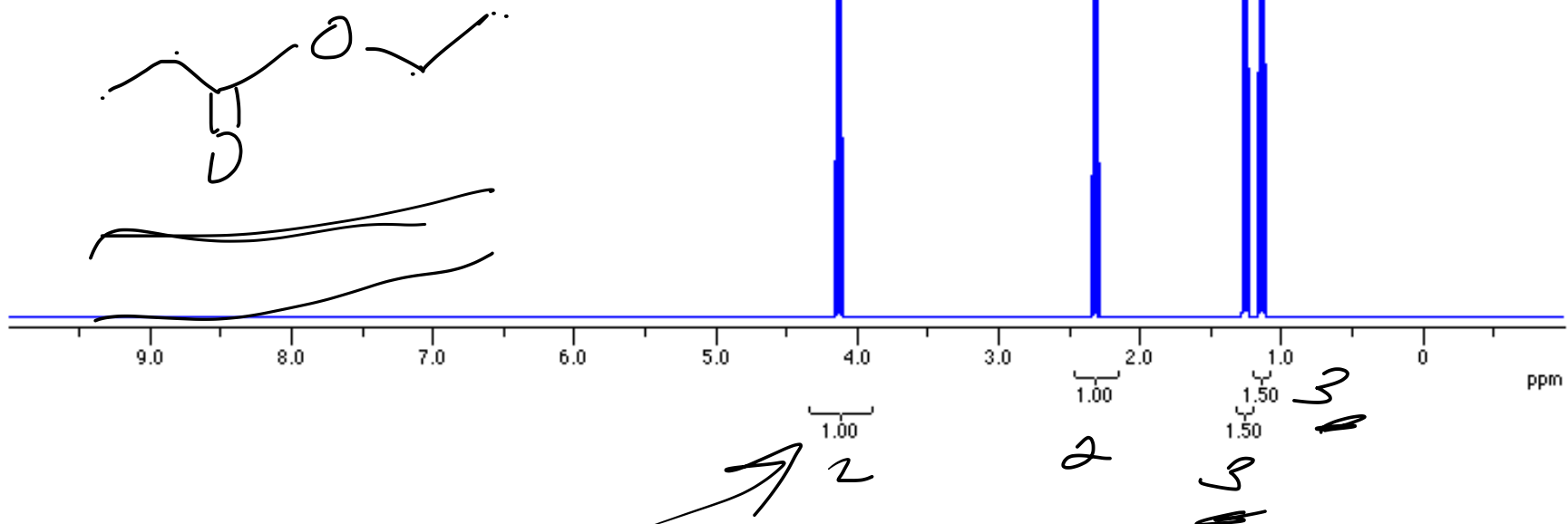
If the number are the same then the area represents the number of H's giving rise to the peak

#H's in formula / # H's in the total area to find the factor to multiply the areas by

$$1 + 1 + (1.5 + 1.5)$$

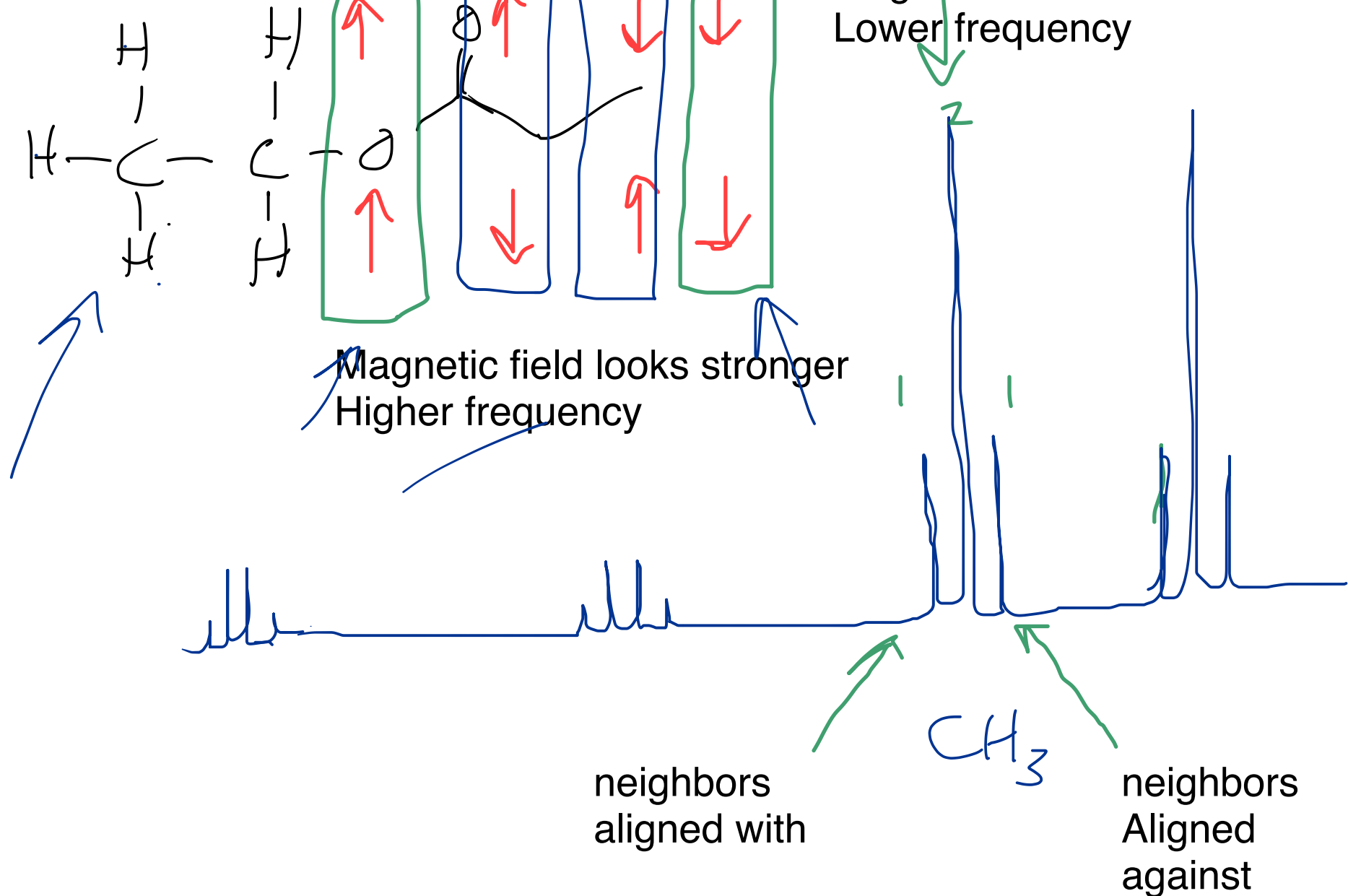
5

$$\frac{10}{5} = 2$$



## Multiplicity

Protons are "coupled" ... scalar, first order coupling, second order coupling is very complicated



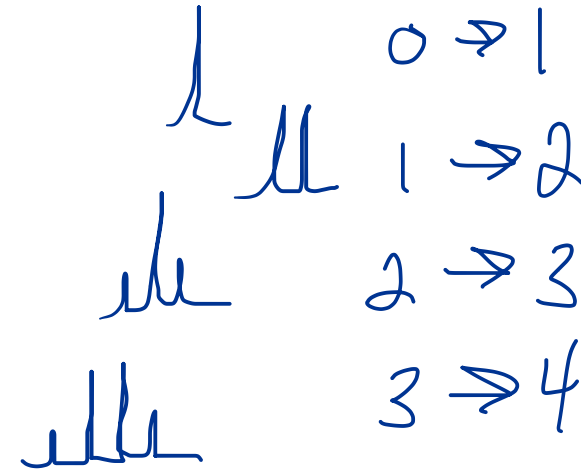
No neighbors... no one to couple with = singlet

One neighbor... 1 H to couple with = doublet

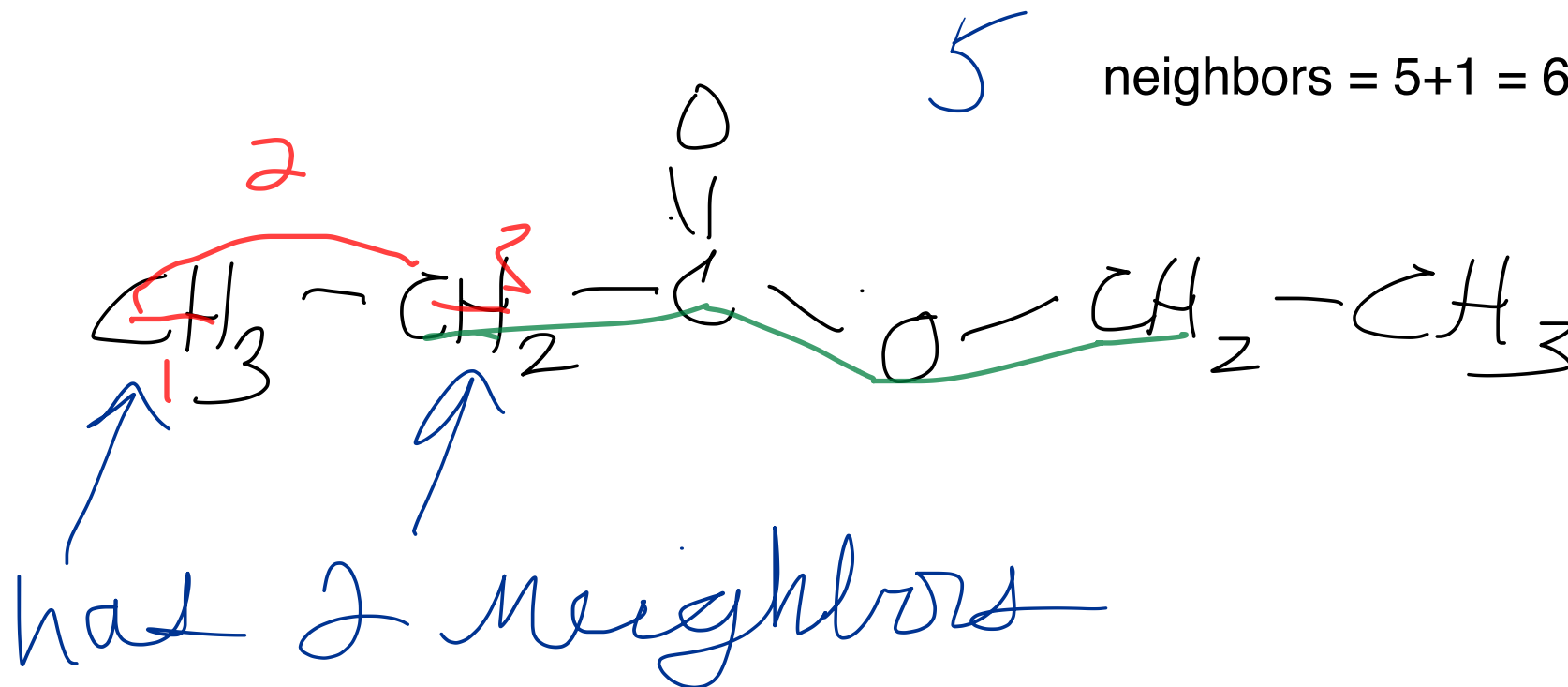
2 neighbors... 2 H's to couple with = triplet

3 neighbors... 3 H's to couple with = Quartet

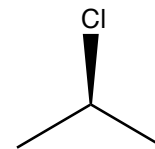
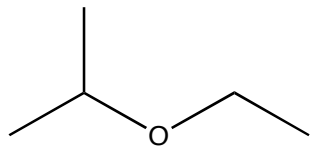
N neighbors gives rise to an n+1 signal



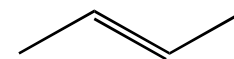
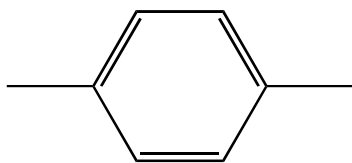
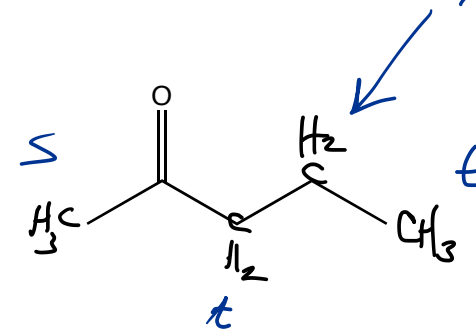
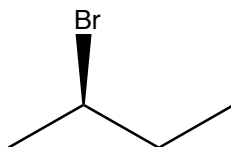
5 neighbors = 5+1 = 6 = sextet



# Determine the multiplicity for the peak on the following molecules



triplet quartet = 12 lines  
 $5 + 1 = \text{sextet}$



Number of different types of H atoms

Chemical environments of the H atoms

How many of each type of H atom

How many H atoms neighbor each different type of H atom