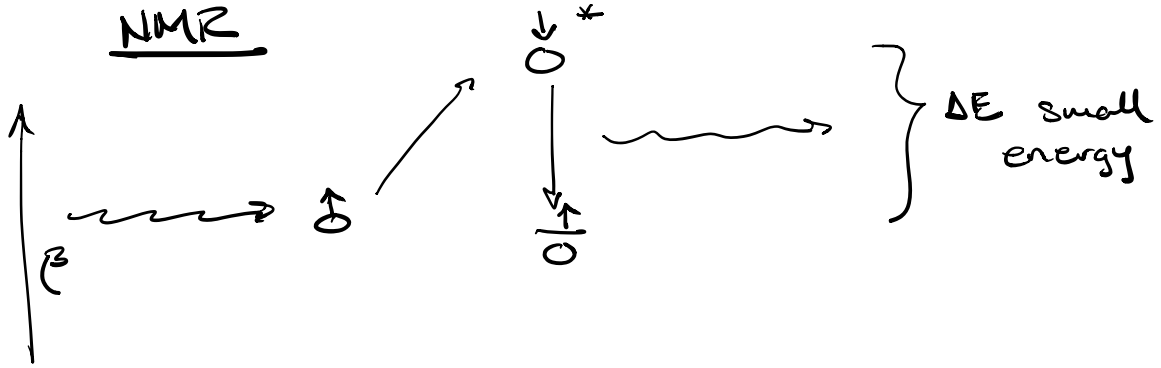
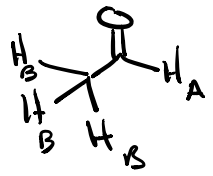
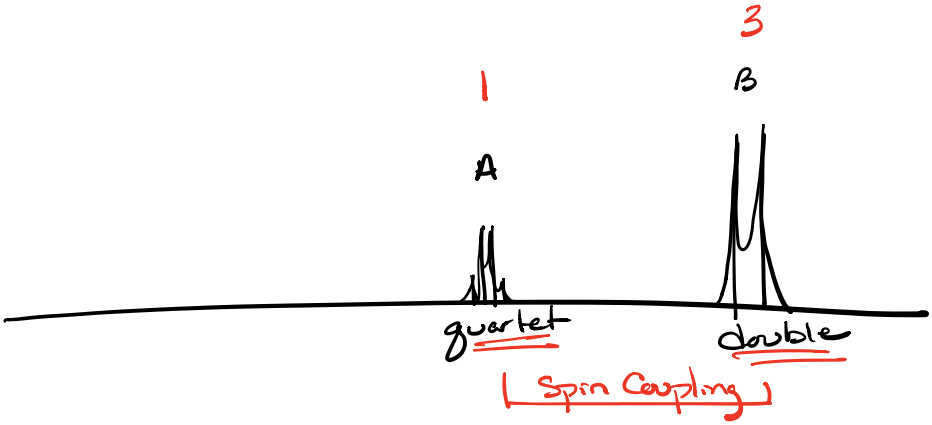
NMR



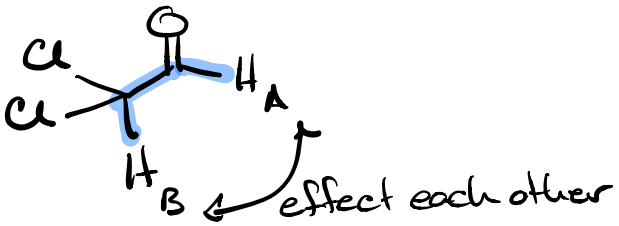
Spin - Spin Coupling



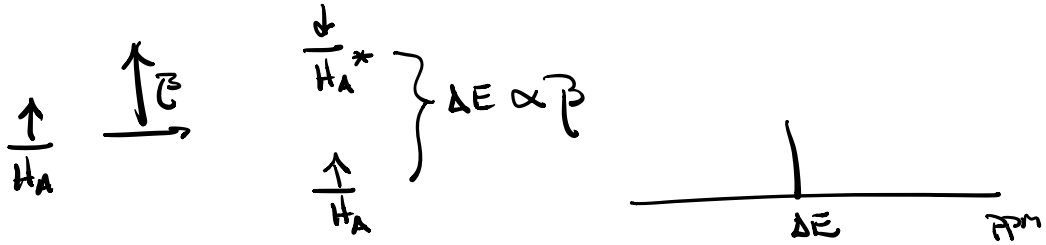
^{1}H-NMR Signals Can be integratable



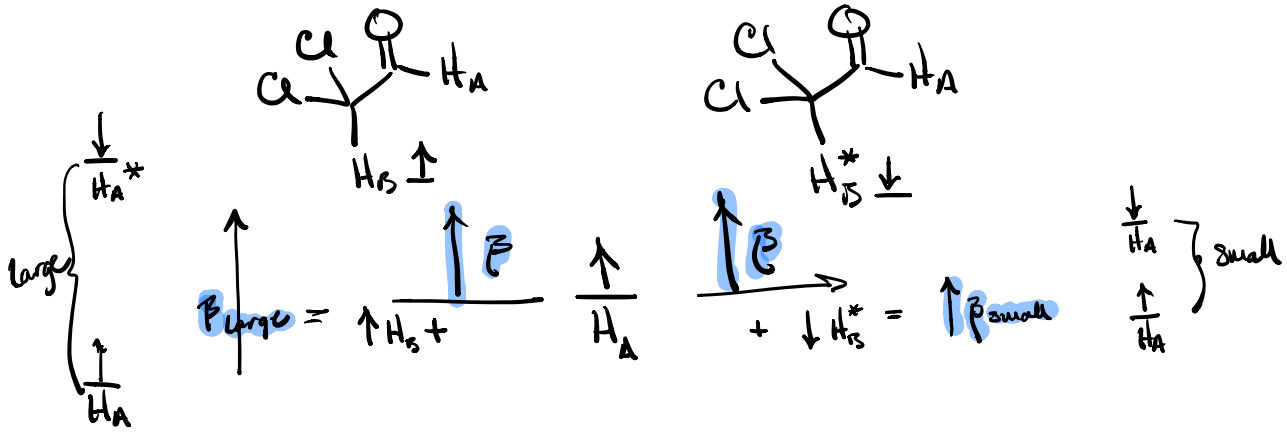
Spin Coupling → Connectivity Information

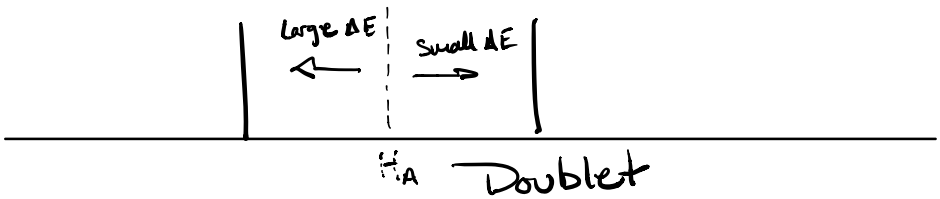


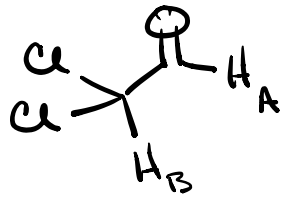
H_A by itself

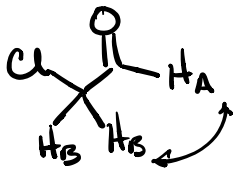


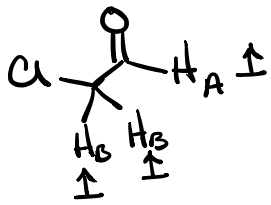
H_A effected by H_B Spin State





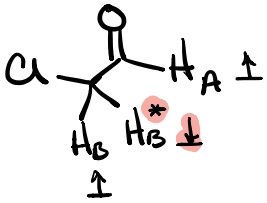


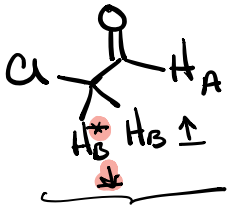




$\uparrow \beta_{normal} + \uparrow + \uparrow =$

$\uparrow \beta_{eff}$ large

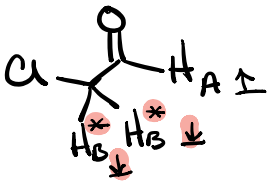




$\uparrow \beta_{normal} + \uparrow + \downarrow$

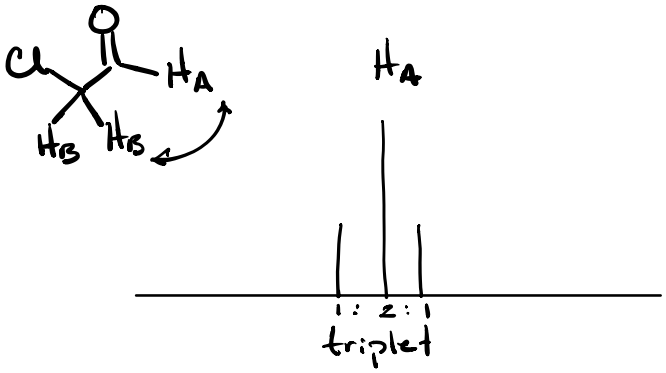
$= \uparrow \beta_{normal}$

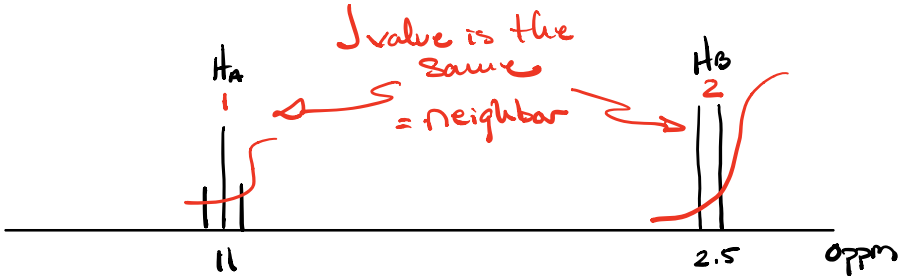
2 ways



$\uparrow \beta_{normal} + \downarrow + \downarrow =$

$\uparrow \beta_{eff}$ = small

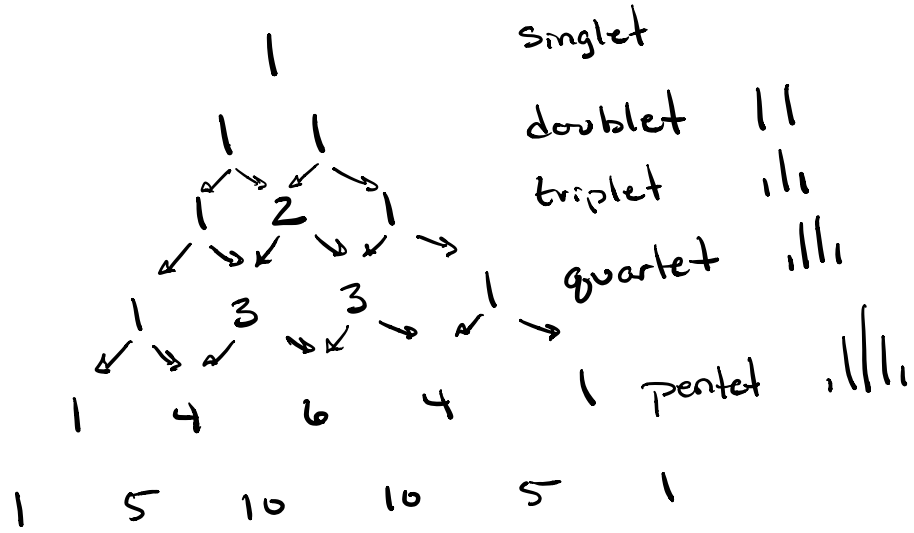


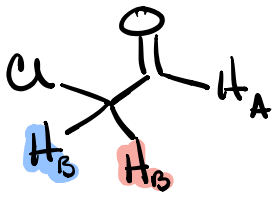


Splitting patterns follow the n+1 rule where n = # of neighbors

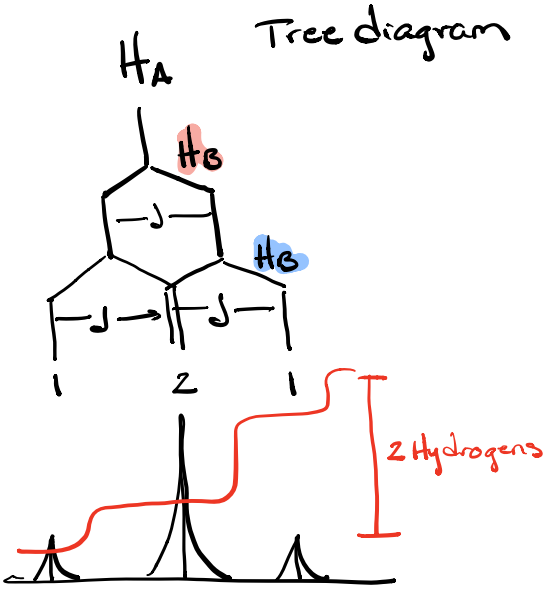
# of neighbors	# Signals (pattern)	
0	1	singlet
1	2	doublet
2	3	triplet
3	4	quartet
4	5	pentet

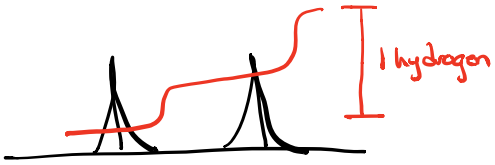
Ratios of lines given by Pascal's Triangle

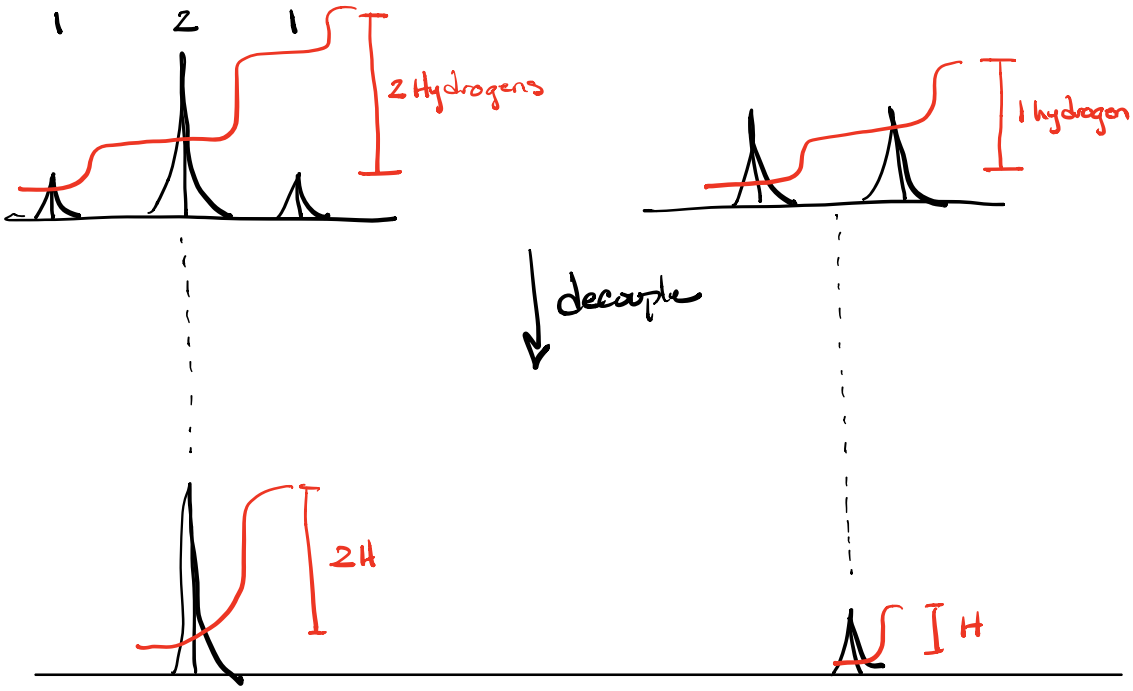


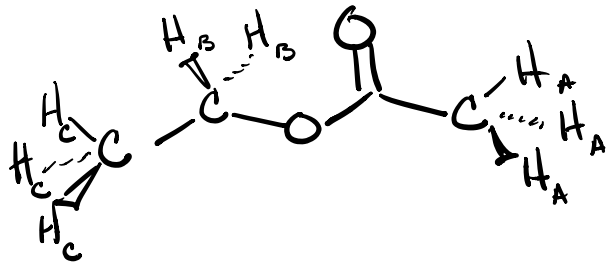


Tree diagram







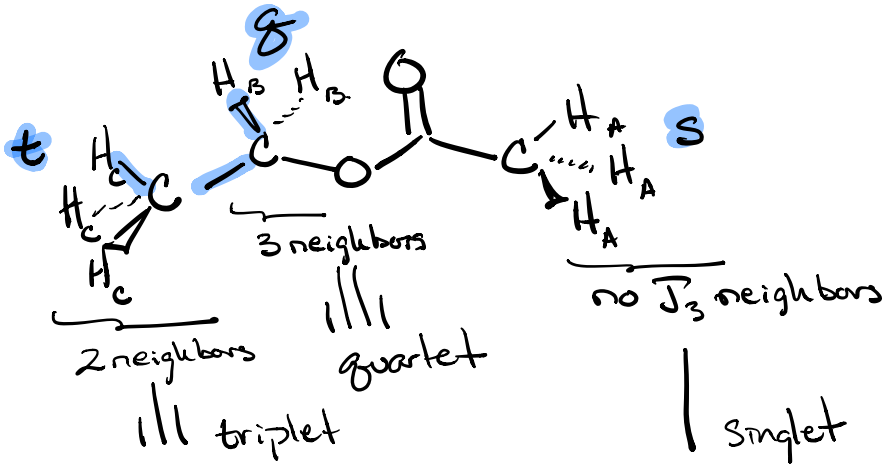


- Protons in same chemical environment do not split each other.

- J described as J_2 or J_3 or J_4 (# of bonds between neighbors)

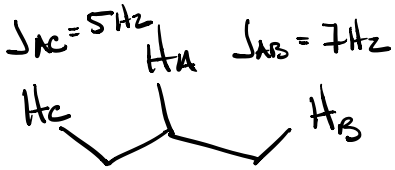
- J_3 are most common

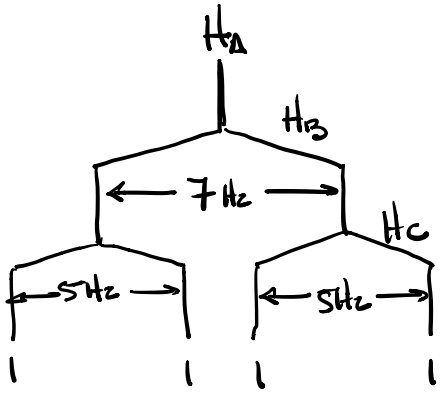
- J_4 & J_5 & J_2 are tiny

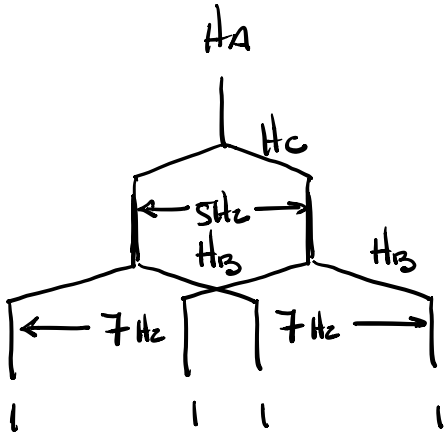


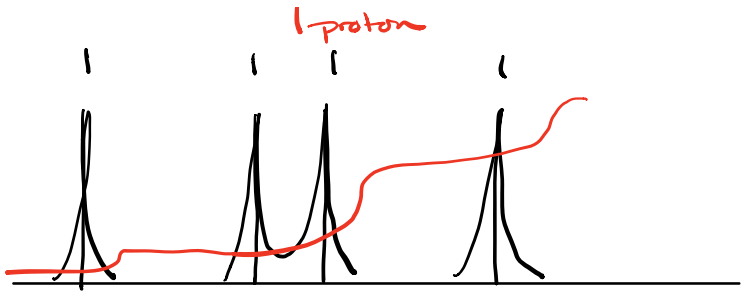
n+1 Rule

# neighbors	pattern	
0	1	singlet
1	11	doublet
2	121	triplet
3	1331	quartet









quartet? 1 3 3 1 No!

double doublet

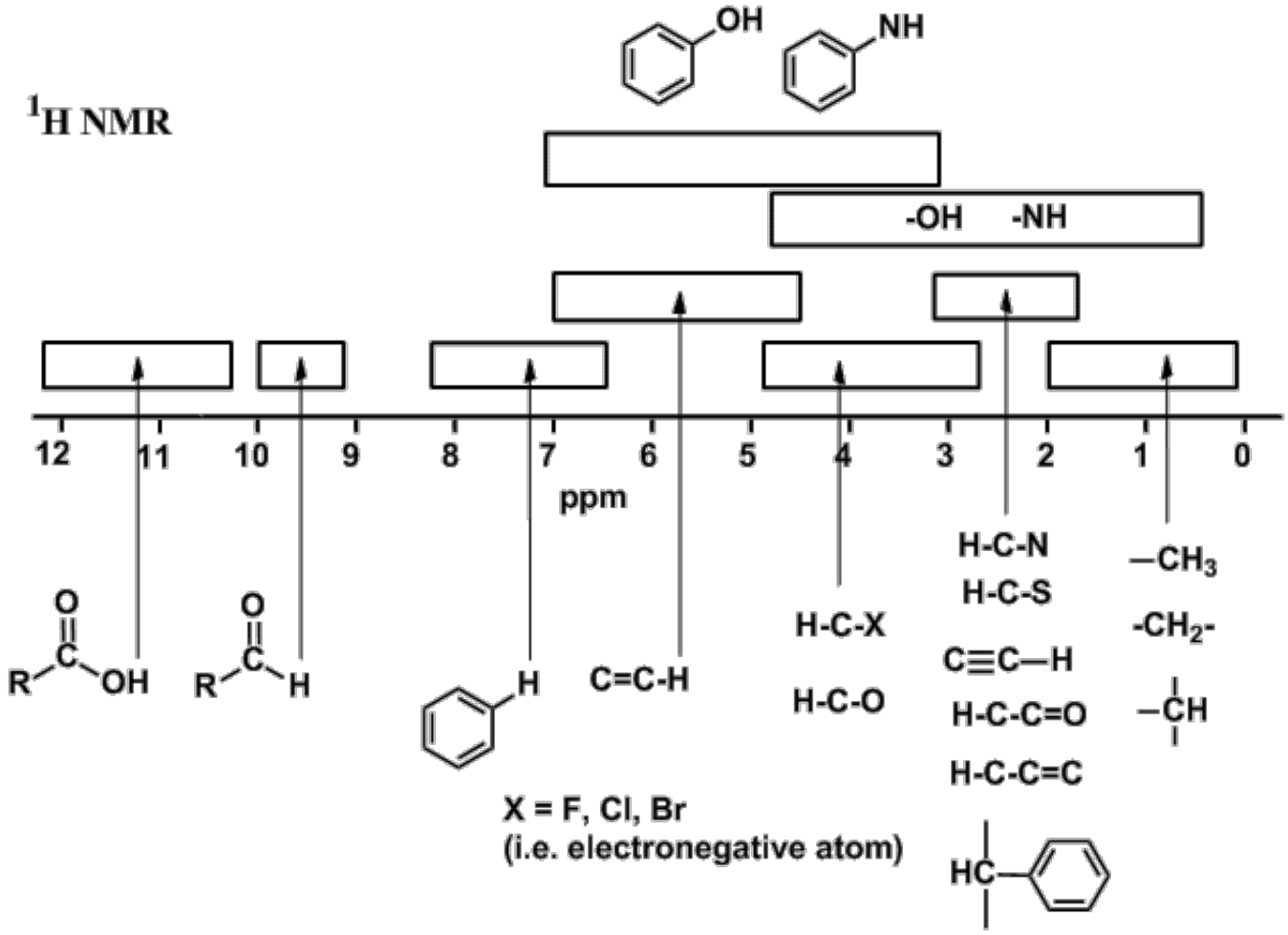
How to analyze Spectra

1. Get a good NMR Table, one for proton & one for Carbon. ⟹ Tables in Pavia are good.
2. Make a table of data

ppm	Integration	Splitting	# of neighbors	Assignment

3. Find the major parts
4. Use neighbors to find connectivity
5. Build possible molecules
6. Eliminate models that don't fit data until a single good model is remaining.

^{1}H NMR


OH
NH
-OH -NH
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
O
C
R
OH
O
C
R
H
H
C=C-H
H-C-X
H-C-O
H-C-N
H-C-S
C≡C—H
H-C-C=O
H-C-C=C
—CH3
-CH2-
—CH
X = F, Cl, Br
(i.e. electronegative atom)
HC

Problem # 1 WebSpectra

ppm	Int	Splitting	# of neighbors	assignment
1.17	3	triplet	2 neighbors	$-CH_3$
1.96	3	Singlet	0 neighbors	$-CH_3$
4.03	2	quartet	3 neighbors	$-CH_2-$

$-CH_3$ s

$-CH_2-CH_3$ q t

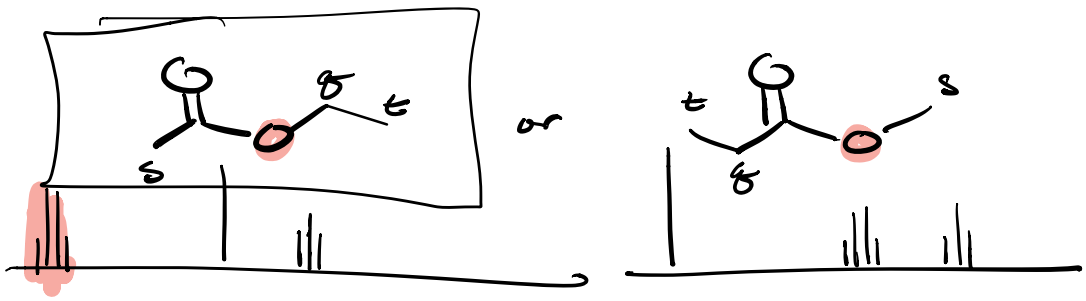
$C_4H_8O_2$

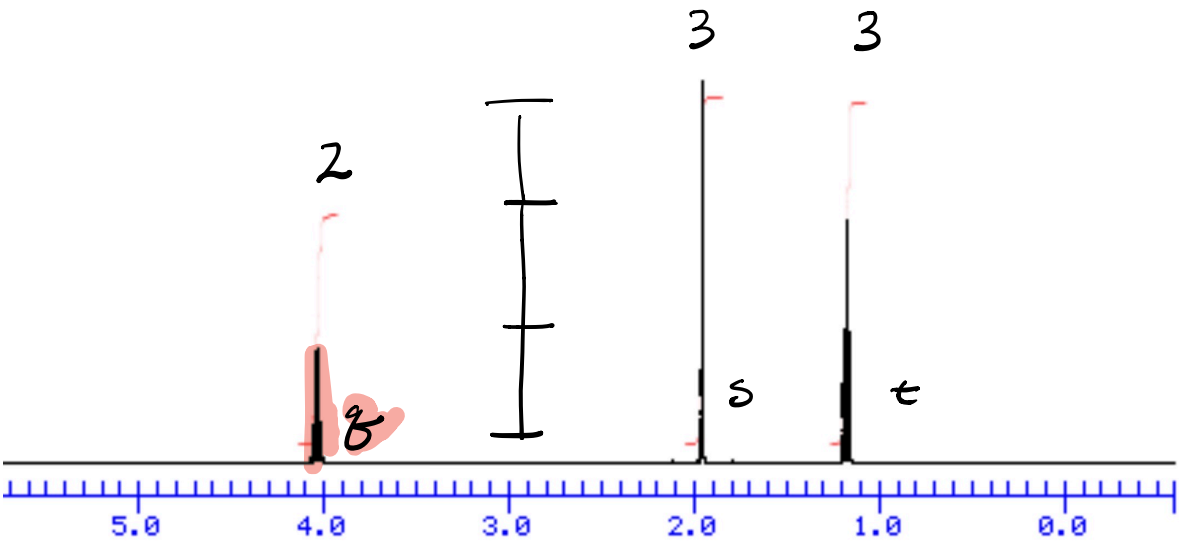
$2x4+2 = 10$

-8

$2|2$

1 unit of unsaturation





Spectrum may be magnified 16X by clicking