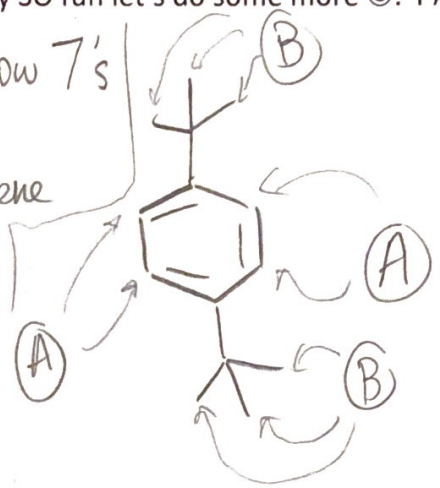
NMR #3: Working with Spectra and Deducing Structures (Part 2)

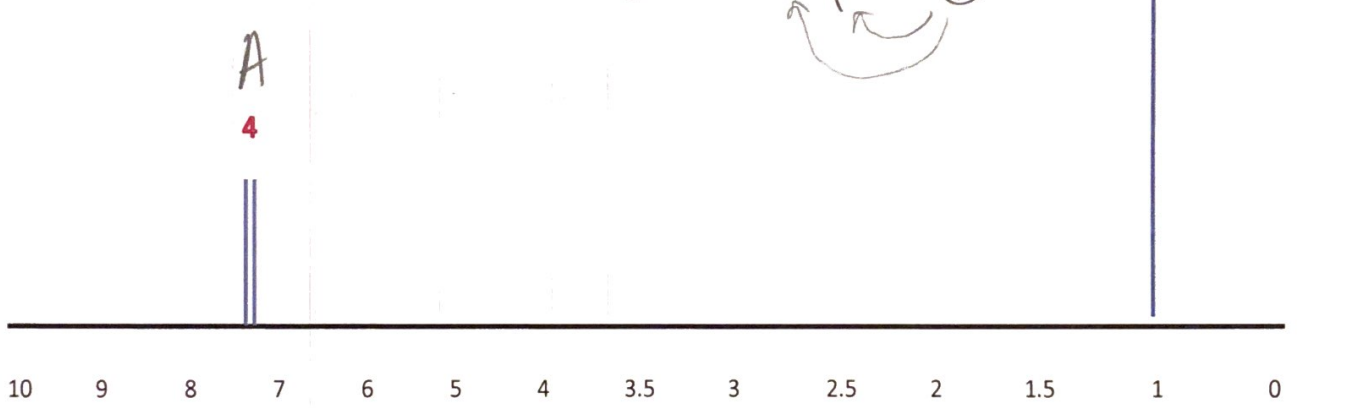
Alright, gang: NMR Part 1 was actually SO fun let's do some more ☺: PART 2 LET'S GO.

- DoU = 4 and chemical shift in low 7's ⇓ Benzene ring

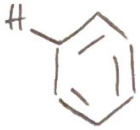
DoU = 4

1.) Molecular Formula: $C_{14}H_{22}$
HNMR Spectrum (below):
Integration #'s are in red



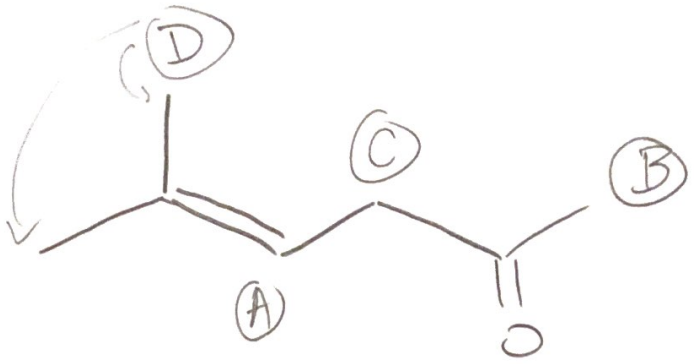


	δ	Coupling	Int.	n	Appearance
A	7.3	doublet	4	1	• aryl H • Symmetry
B	1	Singlet	18	0	• Six $-CH_3$ groups • symmetry • No neighbors

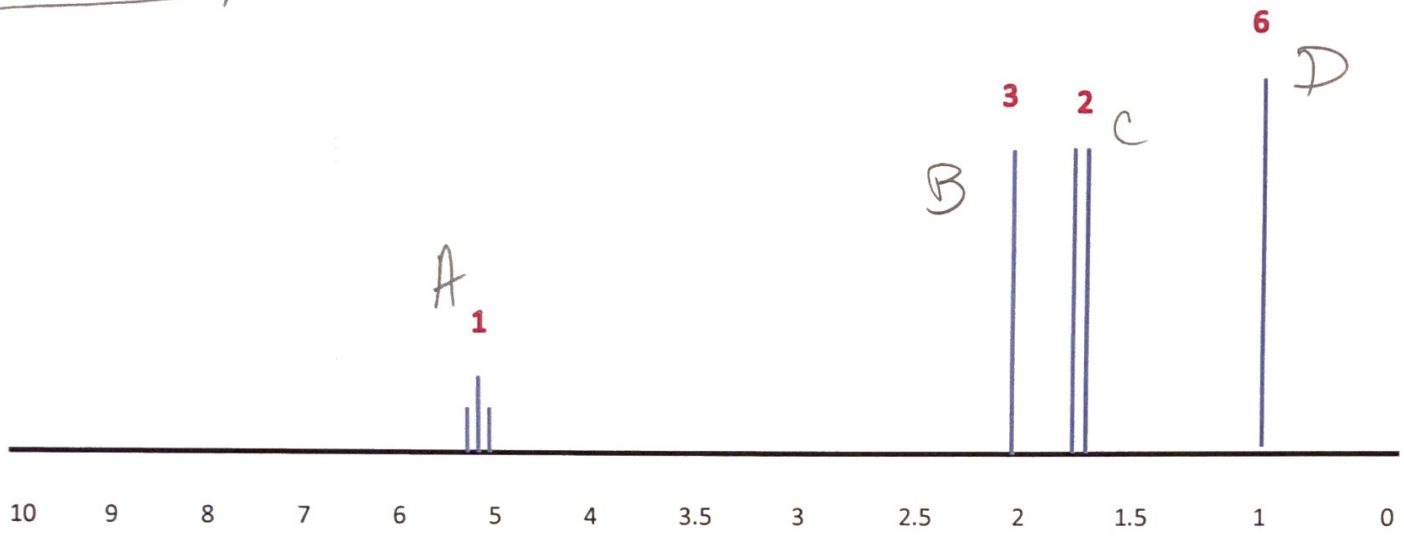


* groups have to be para to have 2 signals/symmetry for signal A

2.) Molecular Formula: $C_7H_{12}O$
HNMR Spectrum (below):
Integration #'s are in red

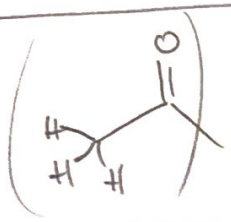
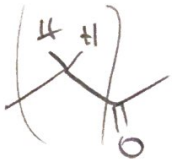
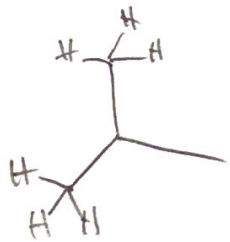


DoU = 2



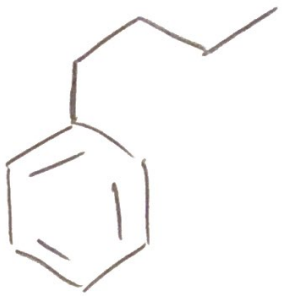
10 9 8 7 6 5 4 3.5 3 2.5 2 1.5 1 0

[PPM]

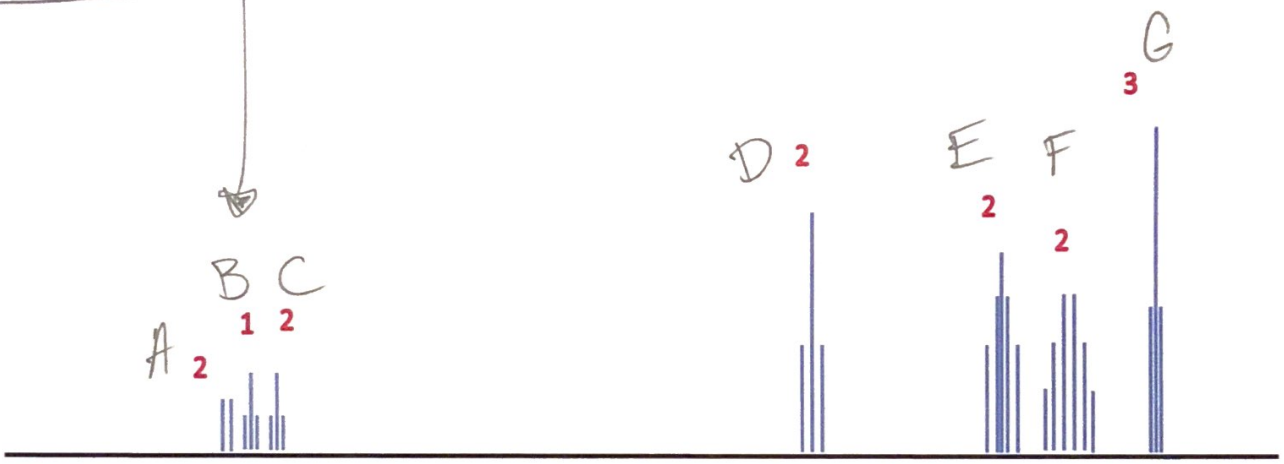
	δ	Coupling	Int.	n	Appearance	
A	5.1	triplet	1	2		"Vinyl" H (which means H of C in a π bond)
B	2.1	Singlet	3	0		• No neighbors • Next to carbonyl • possibly terminal
C	1.7	doublet	2	1		• A little downfield • Next to electronegativ & deshielding things • possibly near carbonyl
D	0.9	Singlet	6	0		• Two terminal $-CH_3$ groups • No neighbors

Benzene Ring

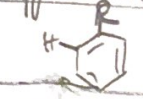
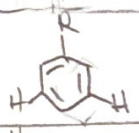
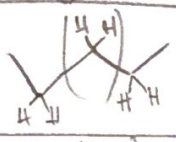
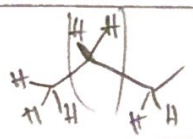
3.) Molecular Formula: $C_{10}H_{14}$
HNMR Spectrum (below):
Integration #'s are in red



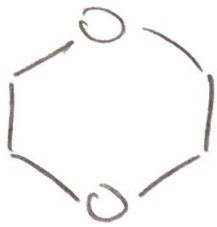
DoU = 4



* Three unique signals from Benzene (5) H's: only one group off of ring

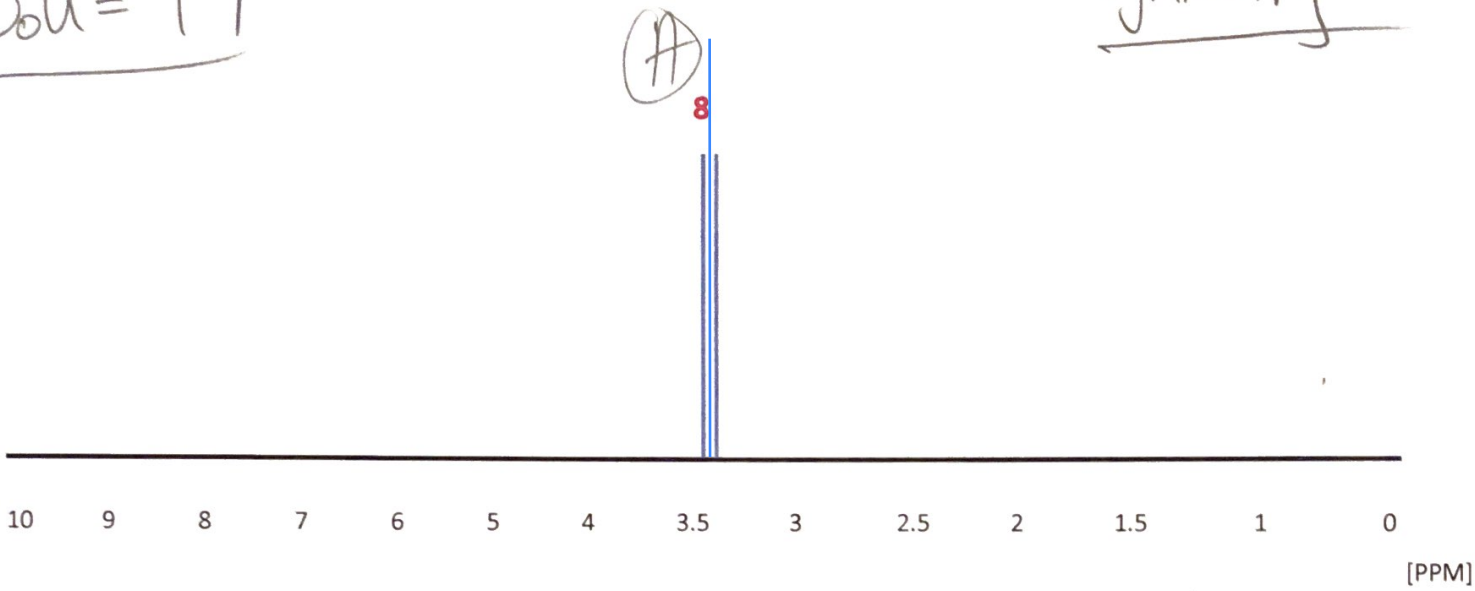
	δ	Coupling	Int.	n	Appearance
A	7.5	doublet	2	1	 • on Benzene ring (aryl H) • 1 neighbor
B	7.3	triplet	1	2	 • on Benzene ring • 2 neighbors
C	7.1	triplet	2	2	 • on Benzene ring • 2 neighbors * symmetry
D	2.6	triplet	2	2	 • In Benzylic position (downfield) • 2 neighbors
E	1.6	quintet	2	4	 • In the middle of a chain • 4 neighbors
F	1.3	sextet	2	5	 • Middle of chain • 5 neighbors
G	0.9	triplet	3	3	 Terminal $-CH_3$

4.) Molecular Formula: $C_4H_8O_2$
HNMR Spectrum (below):
Integration #'s are in **red**



DoU = 1

Symmetry



Ether functional groups