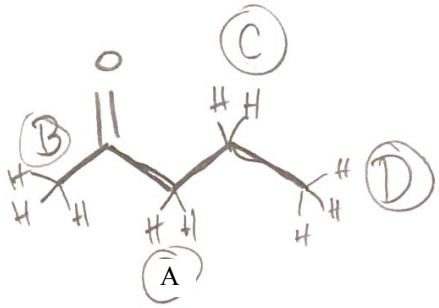
NMR #2: Working with Spectra and Deducing Structures (Part 1)

Alrighty, gang. Now that we have some done some NMR exercises and reinforced the necessary terminology, we've put ourselves in a good position to start tackling problems where you have to deduce structures from HNMR spectra. **Do not get discouraged if you are not good at this at first: I was personally AWFUL.** It took me a lot of practice to get a feel for solving these types of problems—so if you're struggling at first, just remember to not to get frustrated, stay organized, and keep trying. If you're good at them out of the gate, then kudos to you: You've been gifted with a great, coveted gift (not really but that's awesome).

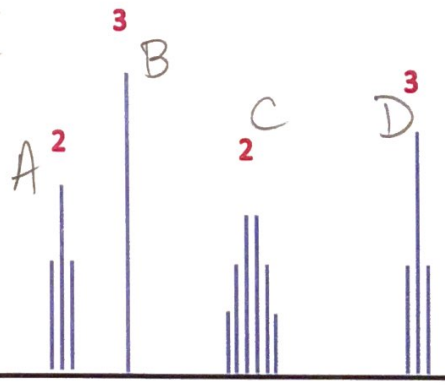
Personally, I like the strategy we discussed in the videos of calculating the units of unsaturation and then making a chart where you write all of the information you can gather about the problem in order to stay organized. However, if you find a better strategy you like better, then by all means, march to your own beat. As long as you can deduce the structure, go for it.

1.) Molecular Formula: $C_5H_{10}O$
HNMR Spectrum (below):
Integration #'s are in red

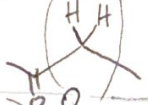


$$DoU = \frac{2(5)+2+0-0-10}{2} = \frac{2}{2}$$

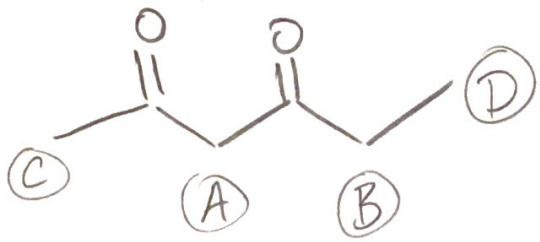
$$DoU = 1$$



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

	δ	coupling	integration #	Neighbors (n)	appearance
A	2.6	triplet	2	2	 downfield
B	2.2	Singlet	3	0	 downfield, terminal w/ NO neighbors
C	1.6	Sextet	2	5	 a little downfield
D	0.9	triplet	3	2	 probably terminal CH_3–

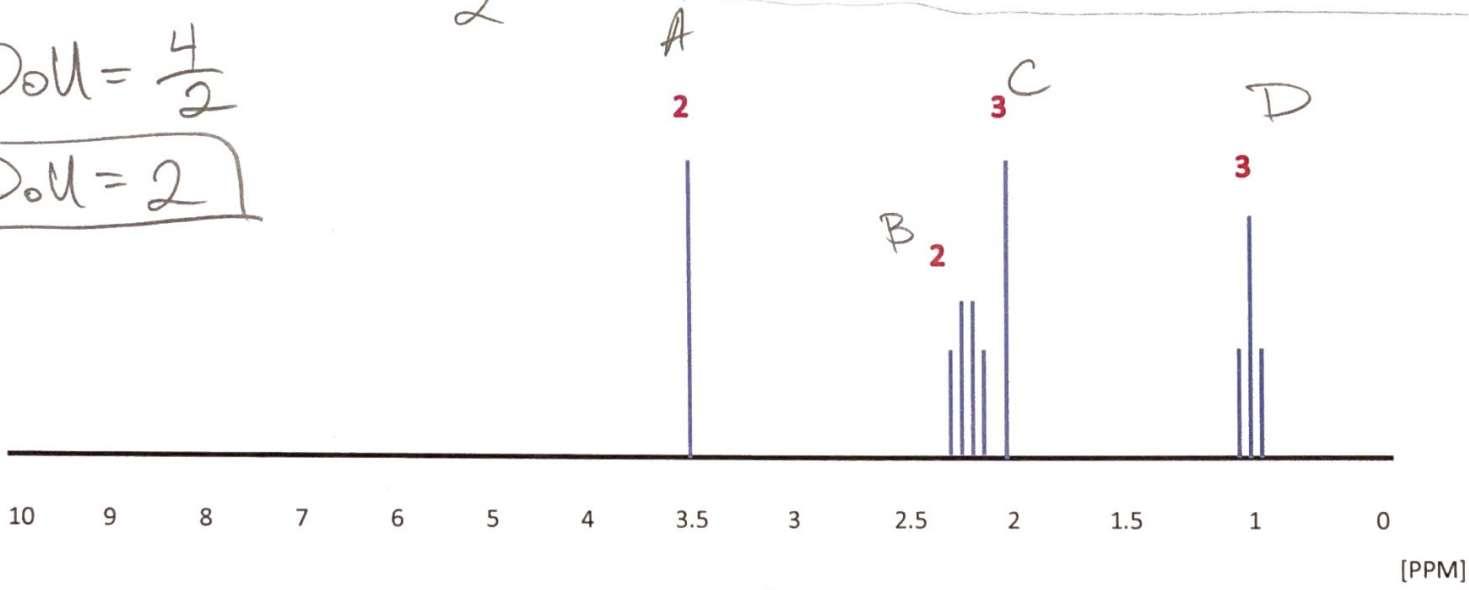
2.) Molecular Formula: $C_6H_{10}O_2$
HNMR Spectrum (below):
Integration #'s are in red

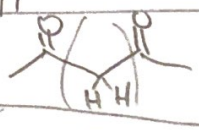
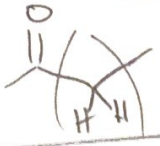
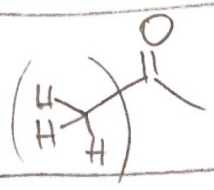


$$DoU = \frac{2(6)+2-0+0-10}{2}$$

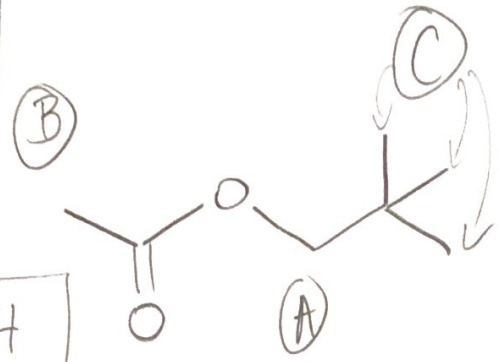
$$DoU = \frac{4}{2}$$

$$DoU = 2$$



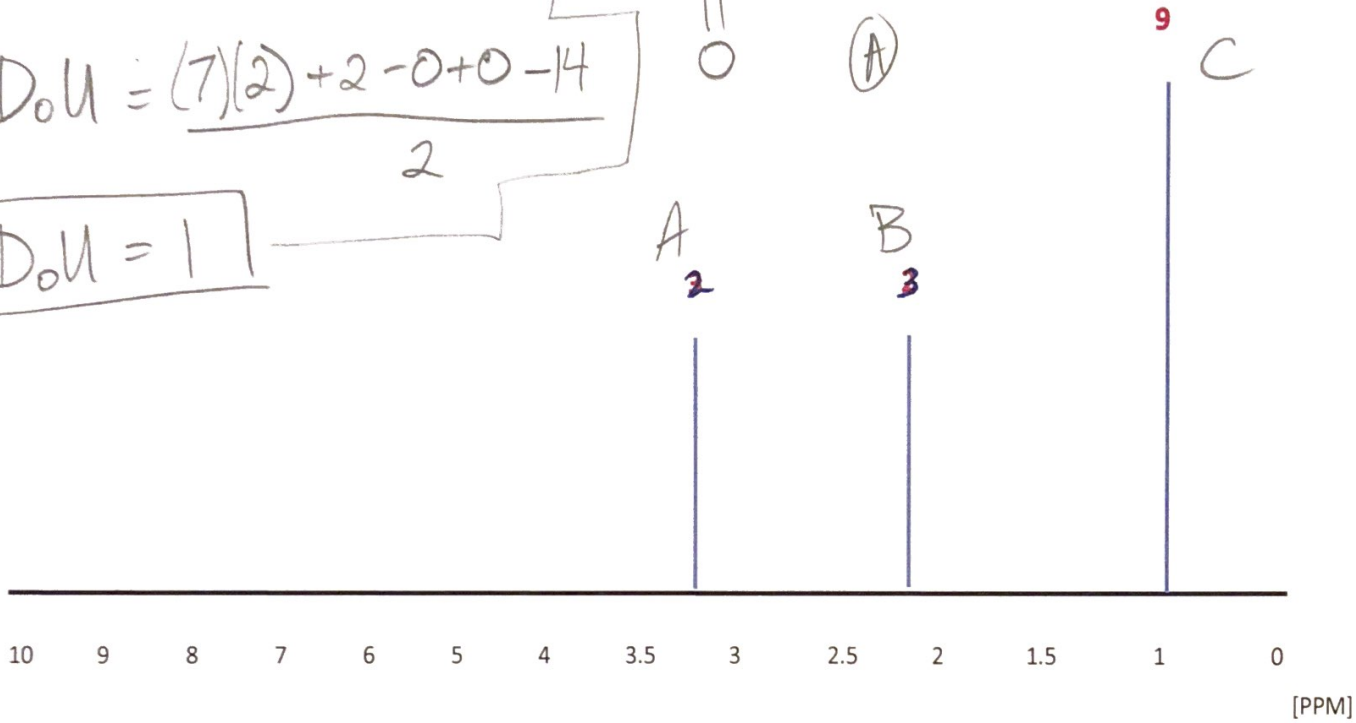
	δ	Coupling	integ.	(n) neighbors	appearance	
A	3.5	Singlet	2	0		★ downfield & No neighbors
B	2.3	quartet	2	3		downfield & has neighbors
C	2.1	Singlet	3	0		★ downfield terminal $-CH_3$ with no neighbors
D	1.0	triplet	3	2		Standard terminal $-CH_3$

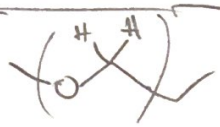
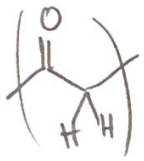
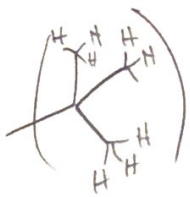
3.) Molecular Formula: $C_7H_{14}O_2$
HNMR Spectrum (below):
Integration #'s are in red



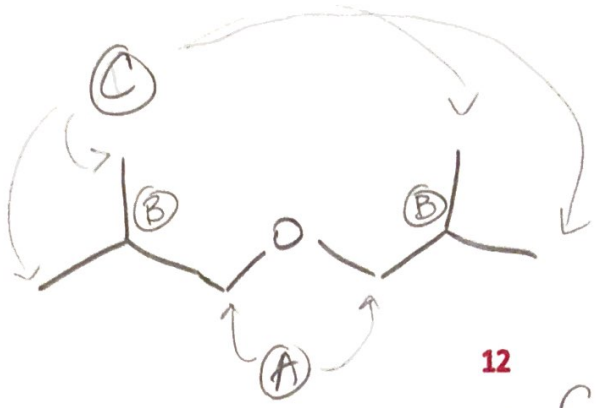
$$DoU = \frac{(7)(2)+2-0+0-14}{2}$$

$DoU = 1$



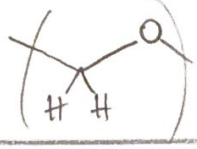
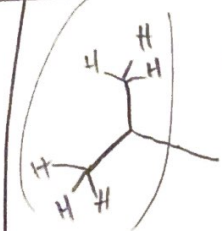
	δ	Coupling	Integ.	(n) Neighbors	Appearance	
A	3.3	Singlet	2	0		• downfield, next to oxygen: Ether • No neighbors
B	2.2	Singlet	3	0		• downfield, next to carbonyl • No neighbors
C	0.9	Singlet	9	0		• Standard $-CH_3$ (three of them) • No neighbors

4.) Molecular Formula: $C_8H_{18}O$
HNMR Spectrum (below):
Integration #'s are in red



$$DoU = \frac{(8)(2)+2-0+0-18}{2}$$

DoU = 0

	δ	Coupling	integration	(n) Neighbors	Appearance	
A	3.4	doublet	4	1		• Downfield • 1 neighbor • ether, 2 of them
B	1.4	nonet	2	8		• A little downfield than normal • Lots of neighbors
C	1.1	doublet	12	1	 ×2	• Standard terminal $-CH_3$: 4 of them • 1 neighbor

* The key to this one is seeing an 8 carbon structure that only has 3 signals: LOTS of symmetry