

**Week 5**  
**CHE 3332 - Organic Chemistry 2**

**Hello and Welcome to the weekly resources for CHE 3332 – Organic Chemistry 2!**

**This week is Week 5 of class, and typically in this week of the semester your professors are covering these topics below.** If you do not see the topics your particular section of class is learning this week, please take a look at other weekly resources listed on our website for additional topics throughout the semester.

We also invite you to **look at the group tutoring chart on our website to see if this course has a group tutoring session offered this semester.** If you have any questions about these study guides, group tutoring sessions, private 30 minute tutoring appointments, the Baylor Tutoring YouTube channel or any tutoring services we offer, please visit our website [www.baylor.edu/tutoring](http://www.baylor.edu/tutoring) or call our drop in center during open business hours. M-Th 9am-8pm on class days 254-710-4135.

**Keywords:** Coupling, Integrating, Chemical Shift

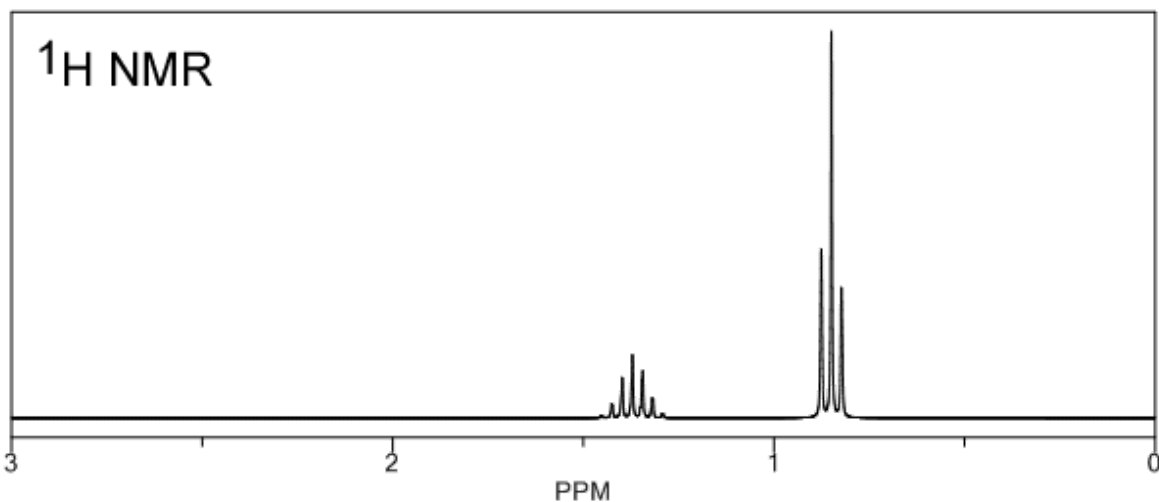
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**TOPIC OF THE WEEK:** Nuclear Magnetic Resonance Imagery (Ch15)

**What is NMR?**

Simply put, NMR is a type of spectroscopy, which detects specific atoms in a molecule, in our case hydrogens (thus we are dealing HNMR). To do so, a large magnet is used, which can flip the hydrogens using magnetically induced poles. Not every atom is capable of doing so, which is why hydrogens are a standard.

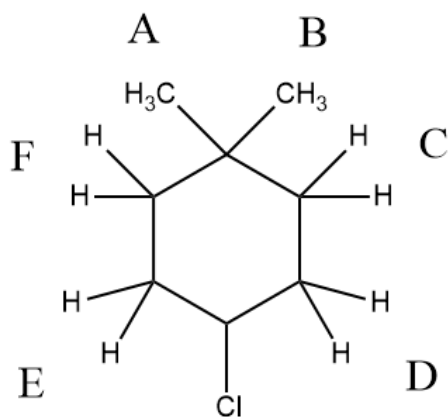
So why do we even need HNMR? Well, if we can properly interpret an HNMR spectra, it can tell us a lot about a molecule, even if we don't know what it is. For example, take a look at the spectra below. Can you figure out what molecule it is showing below? Probably not yet, but we can actually learn a TON about this mystery molecule once we go over HNMR.



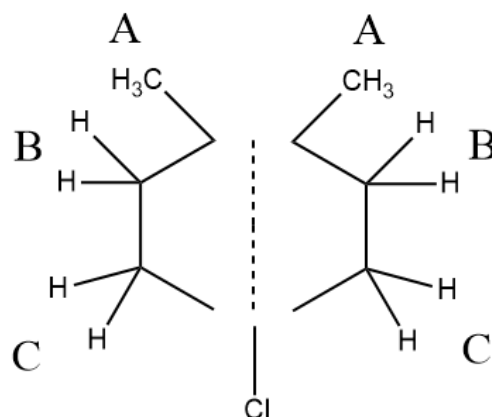
### Symmetry of Molecules:

An important part of HNMR is figuring out how many peaks will show up on the spectra. In order to do so, we must figure out how many unique hydrogen groups there are in the molecule, which we consider chemically independent. Let's use the bottom molecule as an example. From the picture, it can be seen that there are **six** different locations with hydrogens.

**NOTE:** Notice that I say “groups” of hydrogens. That means a CH<sub>3</sub> would only count as one group, not three hydrogens.



Six seemingly unique groups

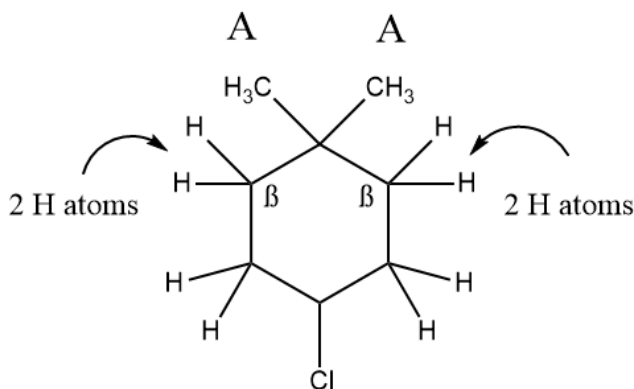


Only 3 are symmetrically different

However, if we were to draw a line through the molecule, splitting it in half, some of the hydrogens are mirrored on both sides. Thus **any hydrogen which is mirrored is NOT chemically independent**. Using this idea as a guiding principle, we can say that there are only **three** independent groups of hydrogens, and we can expect six peaks to show up.

### Coupling & Multiplicity:

Notice how on each signal in the spectra above, that there are smaller peaks which make up the overall signal. This is due to how the hydrogens interact with each other. For your class, it is important to know that the amount of smaller peaks corresponds to the number of hydrogens neighboring our original hydrogen. For example, let us look at our molecule again, specifically at group A.



If we take a look at all the hydrogens present on the neighboring carbons (or beta carbons), we can see that there are **FOUR** neighboring hydrogens. Thus our signal for our group A will have **FIVE** peaks; one for the original group, and the other six for the neighboring hydrogens. If we were to have a group with no adjacent hydrogen atoms, then it would simply show up as a single long peak.

### Chemical Shifting:

Another important topic involving HNMR is the concept of chemical shifting, in relation to the ppm, which constitutes the units on the X axis. Shifting can occur depending on what substituents our hydrogen groups are close to. Specifically, those which are electronegative will shift the ppm over to the **LEFT** which will **INCREASE** ppm. This is due to the withdrawal of electrons towards the more electronegative element, decreasing electron shielding of the neighboring atoms, like hydrogen.

Using our molecule again, the groups labeled C would be the most impacted by the chlorine atom, and would have a **higher ppm** in comparison to the other groups. As we get farther away from the chlorine, the ppm shift will have a lesser effect on each hydrogen group.

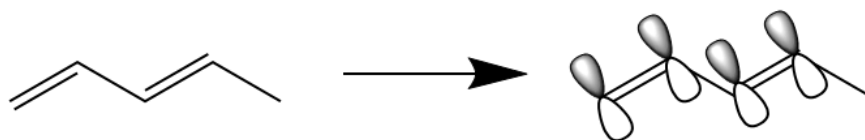
### Here are some common players in shifting ppm:

Substituent	Chemical Symbol	Shift in ppm
Methyl	R-CH <sub>3</sub>	0.9
Alcohol	O-H	~2.5

Alkyl Halide	H-C-X	~3
Vinylic	C=H	~5
Carbonyl	O=C-H	~10

### HIGHLIGHT #1: Conjugated Pi Systems

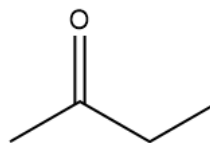
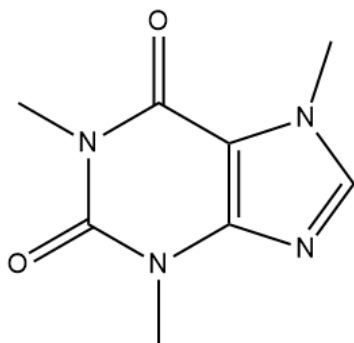
Because you all will likely not be covering too many topics this week, we will just get slightly ahead, and talk about the next chapter a bit just to familiarize ourselves with it. So to begin with you may be thinking, what are conjugated systems anyways? Simply put, these are systems formed from the pi (or double bonds) being in close proximity to each other.



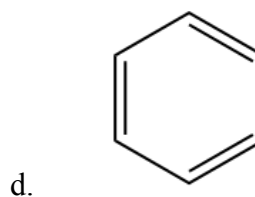
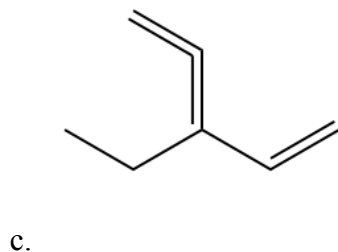
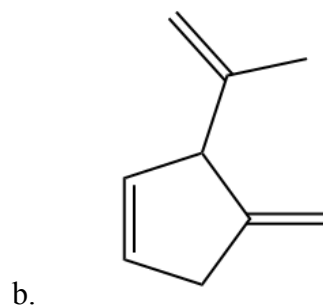
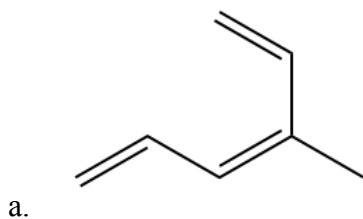
If the pi bonds are properly spaced on a molecule, such as the one shown above, we can say they are conjugated, and will thus boost the stability of the molecule. Any pi bonds which are either right next to each other, or perhaps too far apart, will not participate in conjugation. Additionally, all the p-orbitals must be in phase with each other. Without this, the bonds would not have their pi bonding characteristics.

### CHECK YOUR LEARNING:

For the following molecules, how many peaks, and coupling peaks would be present?



For the following molecules, determine if they will or will not have a conjugated pi system:



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### THINGS YOU MAY STRUGGLE WITH!

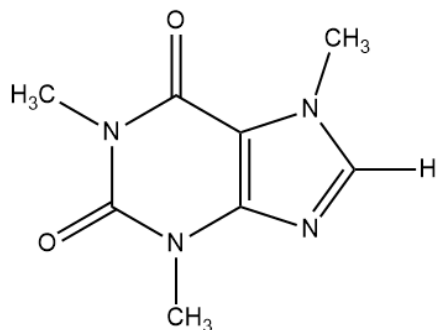
- For HNMR, something I always found tricky was being able to determine if two groups of hydrogens were chemically identical or not. It is always a good idea to practice, and this should be something that I would pay attention to.
  - In a similar vein to the last point, I would also focus on keeping track of counting **groups** (for the # of signals), and counting the **individual** hydrogens (coupling). Sometimes you might mix them up on accident
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Thanks for checking out these weekly resources!

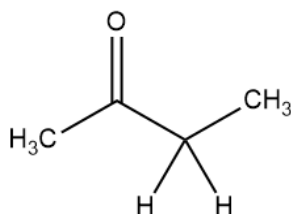
Don't forget to check out our website for group tutoring times, video tutorials and lots of other resources: [www.baylor.edu/tutoring](http://www.baylor.edu/tutoring)! Answers to check your learning questions are below!

### Answers for practice problems:

1. Looking at the first molecule, which is caffeine, we can see that it has four distinct groups of hydrogens that are not symmetrical.



Additionally, no group has any neighboring beta hydrogens next to them, thus each peak will show up as a single peak (a singlet). Additionally, because of the carbonyl groups, the two CH<sub>3</sub> groups on the larger six sided ring will likely be shifted greatly to the left.



For our next molecule, butanone, we can see that there is no symmetry of the molecule, making each hydrogen group chemically distinct for our purposes, and giving us three peaks on our spectra. In regards to the coupling, the CH<sub>3</sub> to the left has no neighboring hydrogens, and will appear as a singlet. However, the two hydrogens, and the CH<sub>3</sub> are right next to each other. Thus, for the 2H portion, it will be a quartet signal (4 peaks) due to the three adjacent hydrogens. Likewise, for the CH<sub>3</sub> it will be a triplet peak (three peaks) due to the two neighboring hydrogens.

2.

- For a, each double bond is spaced evenly and are all in a continuous line, thus, it will have a conjugated system.
- For molecule B, neither double bond is within one carbon of each other, and are spaced too far apart, negating the possibility of conjugation.
- Notice how for molecule C, it has two double bonds at the top, which are right next to each other. Because of this spacing that is too close, these would not participate in a conjugate system.
- Finally for benzene, similarly to the last molecule, each double bond is spaced out evenly in a ring, and will always be conjugated.

*All tables are property of Organic Chemistry by David Klein. The HNMR spectra is provided by the University of Sydney, Australia. All drawings of molecules and mechanisms are made by me.*