

Week 4 CHE 3332 - Organic Chemistry 2

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

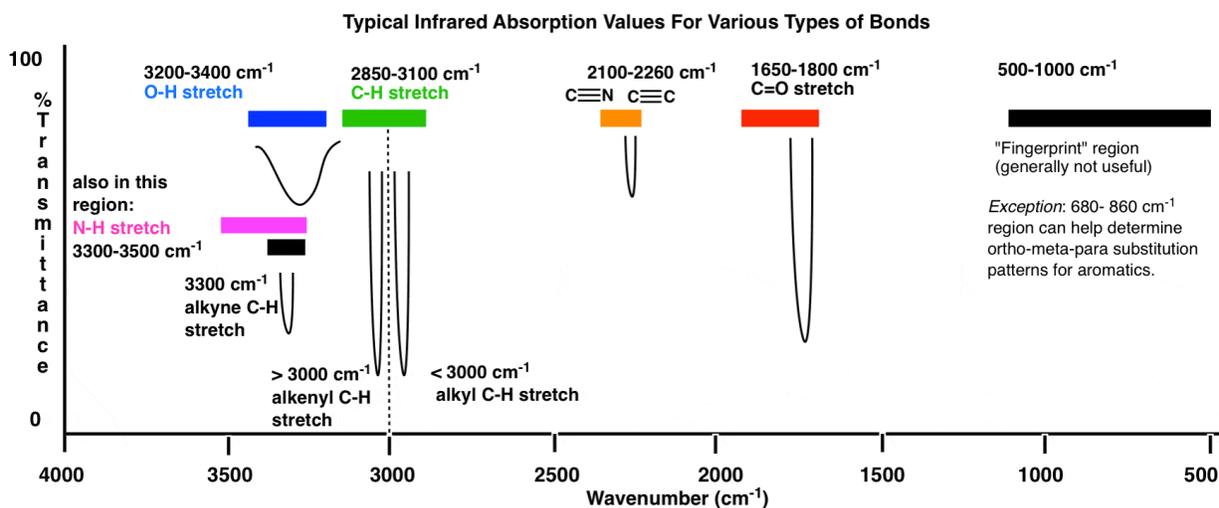
This week is **Week 4 of class**, and typically in this week of the semester your professors are covering these topics below. If you do not see the topics your particular section of class is learning this week, please take a look at other weekly resources listed on our website for additional topics throughout 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 or call our drop in center during open business hours. M-Th 9am-8pm on class days 254-710-4135.

Keywords: Infrared Spectroscopy, Mass Spectrometry, Hydrogen Deficiency Index, Unsaturation

TOPIC OF THE WEEK: Spectroscopy & Spectrometry (Ch. 14)

What are IR Spectra in Ochem, and what do they tell us?



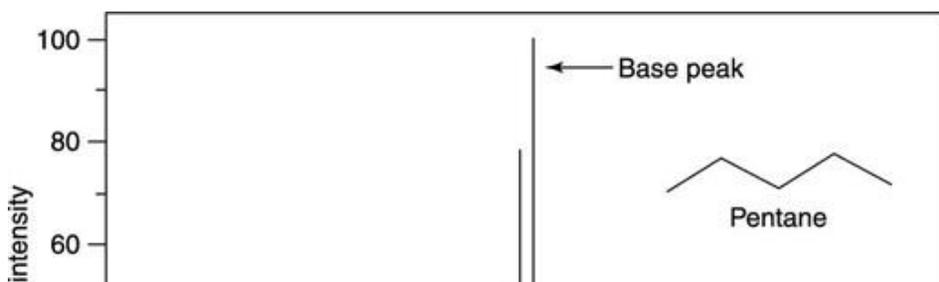
IR Spectra are graphs that help to tell us the characteristics of a molecule, namely which functional groups it has. To do so, it uses infrared radiation to vibrate the bonds between two atoms, with each pair of two different atoms having its own distinct vibration. On an IR spectrum, these vibrations will show up as peak, pointing downwards. The units on a spectrum are in inverse centimeters, so as the graph moves to the **right**, the numbers get **smaller**.

The main use of IR spectra is to be able to tell what function groups are in a molecule, without even looking at it. For example, if you were to see an IR spectra containing signals for a carbonyl bond, you would know that your molecule is likely a ketone (or aldehyde)/ For your Ochem class, it is most important to learn which values correspond to which functional groups.

Important Functional Groups:

MEMORIZE THESE!!!

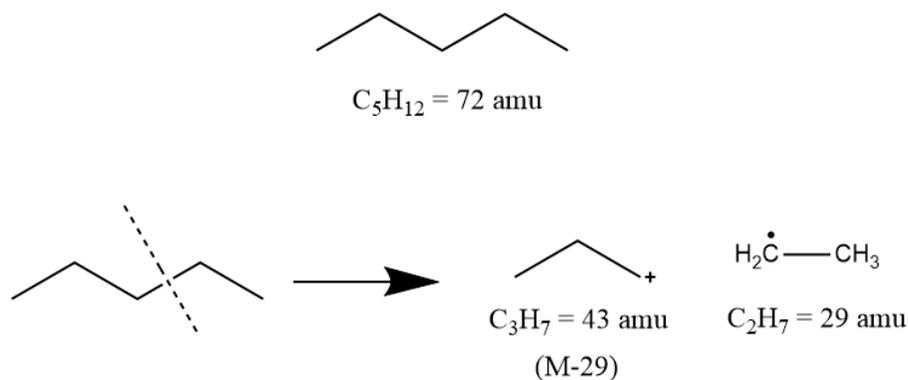
Bond	Wavenumber (cm ⁻¹)	Shape
C=O (Carbonyl)	Around 1750	Thin and long peak
O-H (Hydroxyl)	3000-3400	Long and broad, usually encompasses the whole range
C-H (Alkane)	3000	Thin and sharp peak, always present
C=C (Alkene)	3000-3200	Similar in shape to alkanes
C≡H (Alkyne)	3300	Similar in shape to alkanes
Benzene	Around 1650	Series of small bumps
C≡C (Alkyne)	2100-2200	Medium size and length of peak
C≡N (Nitrile)	2200-2300	Similar in shape to C≡C
N-H (Amine)	Around 3400	Small broad peak, maybe have multiple peaks for each hydrogen connected to nitrogen



What is Mass Spectrometry?

Mass spectrometry is a procedure where a molecule is predictably fragmented, leaving behind an analyzable **mass spectra** which can give information about the parent molecule.

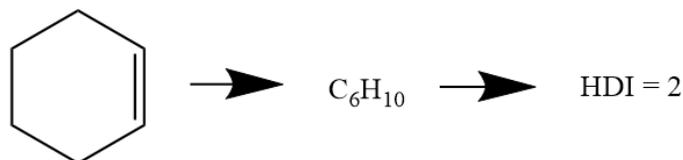
The fragmentation of molecules is usually very predictable, and follows general patterns. For example, using pentane, it is very likely to fragment into two pieces (both a 3 and 2 carbon molecule).



Usually, the fragment with the positive charge is the one that is analyzed and added to the spectra. Also note that the nomenclature used for that fragment is M-29, indicating that it is 29 amu lighter than our parent molecule.

HIGHLIGHT #1: Hydrogen Deficiency Index and Degrees of Unsaturation

One final metric we can use to help determine the structure of the molecule is its Hydrogen Deficiency Index (HDI). As the name suggests, this tells us how many hydrogen atoms are missing from a molecule, due to ring structures and π bonds (double or triple bonds).



For example, looking at the structure above, we can see that it is a ring structure (cyclohexane) and contains a single double bond, thus it will have an HDI value of 2. For every increase in HDI, a molecule will lose 2 hydrogens. In the case above, while a normal 6 carbon chain would have 14 hydrogens, the molecule has only 10 hydrogens.

While HDI is simple in its application, it is a bit limited, so we can also find the degrees of unsaturation of a molecule, which gives us similar information about a molecule. It makes use of any nitrogens and halogens present in the molecule too. The equation is as follows:

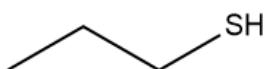
$$(2C + 2 + N - H - X)/2$$

In this equation; C = Carbon, N = Nitrogen, H = Hydrogen, and X = Halogen

NOTE: As seen in the equation, oxygen has no bearing on unsaturation!

HIGHLIGHT #2: Thiols and Sulfides

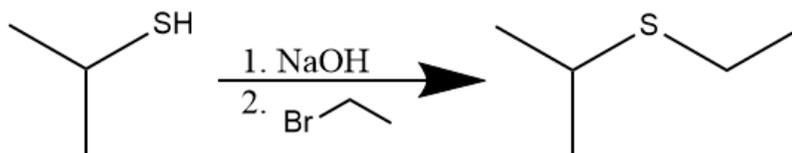
Thiols are just like alcohols, except that they have an -SH group, instead of an -OH group.



Propanethiol

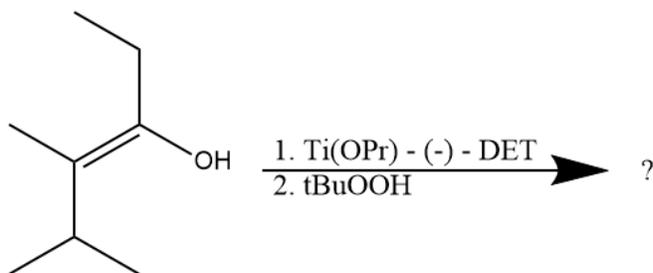
Important: Thiols have similar properties to alcohols, but are much stronger. Thus, they are both more acidic, and function as a great nucleophile.

Additionally, since going from an -OH to an -SH substituent would yield a new classification of molecules, it would be reasonable to expect that an ether (R-O-R), would become a different type of molecule when the central oxygen is replaced with a sulfur (R-S-R). We can call these molecules molecules thioethers. To synthesize these molecules, we can basically just perform a Williamson Ether Synthesis, while using a thiol as our nucleophile.

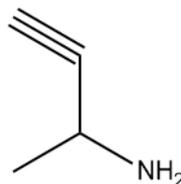
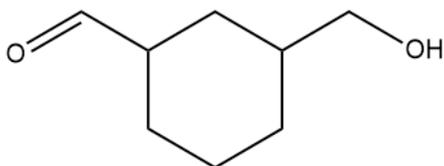


CHECK YOUR LEARNING:

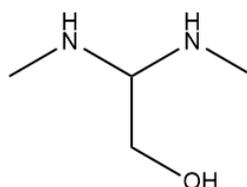
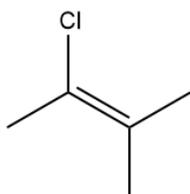
1. Predict the product for this reaction:



2. What IR spectra peaks would be likely to show up for each of these molecules?



3. Find the degrees of unsaturation for the following molecules:



THINGS YOU MAY STRUGGLE WITH!

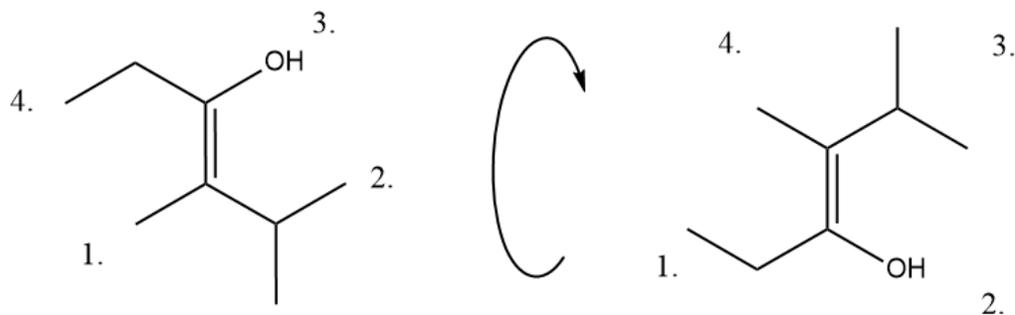
- Naming conventions for all the different molecules can be a bit confusing at times considering how many types there are. If you can get them down, it will definitely help you during the test, and will be free points.
- Similarly to last time, remember to keep up with your Ochem 1 knowledge! As we continue on with the semester, many reactions will build off of material from Ochem 1, so remember to keep those topics up to date.

Thanks for checking out these weekly resources!

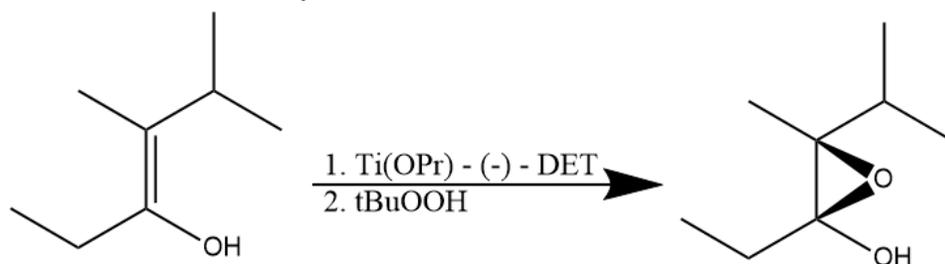
Don't forget to check out our website for group tutoring times, video tutorials and lots of other resources: www.baylor.edu/tutoring! Answers to check your learning questions are below!

ANSWERS FOR PRACTICE PROBLEMS:

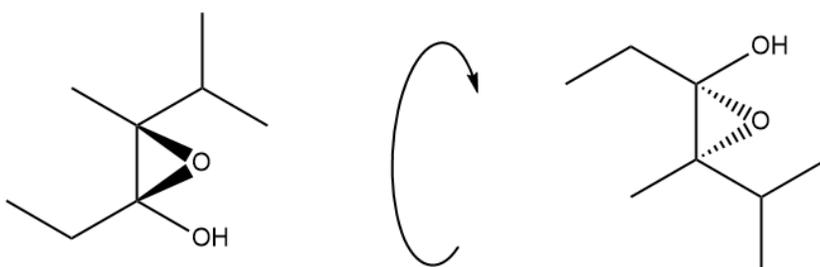
1.



Starting by aligning the hydroxyl to be in the bottom right position. This is something that should be done for every SAE reaction.



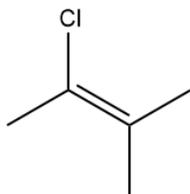
Secondly, once the hydroxyl is in place, you can perform the reaction.

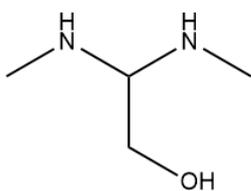


Finally, rerotate (and in this case flip) the molecule back to its original position.

2. For the first molecule, we can identify both a carbonyl (C=O) and an alcohol (O-H) bond. Thus we expect there to be two signals, one at $\sim 3200\text{ cm}^{-1}$ and one at $\sim 1700\text{ cm}^{-1}$. For the second molecule, we can see a triple bond (C \equiv C) as well as an amine (N-H), so we expect both a peak at 2200 cm^{-1} and one $\sim 3400\text{ cm}^{-1}$.

3. This molecule has 5 carbons, 9 hydrogens, and a single chlorine. Using the equation provided above, this would give us an unsaturation of: 1





This molecule has 4 carbons, 12 hydrogens, 2 nitrogens, and an oxygen.
Using the equation above, the unsaturation would be: 0



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