

Week 8

CHE 3331- Organic Chemistry

This week is Week 8 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 of 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: Substitution Reactions, Nucleophile, Electrophile

TOPIC OF THE WEEK: SUBSTITUTION REACTIONS

Last week, we introduced substitution reactions and gave you a few details on how to differentiate between SN1 and SN2 reactions. This week, we will be going in more depth on how to differentiate between both reactions and some key tips for learning how to approach them!

- What is a substitution reaction? This type of reaction occurs when a nucleophile “swaps” places with an electrophile, either in one step or in multiple steps.
 - It is important to understand what words mean before we start defining reactions
 - An **electrophile** is a substrate that is “electron loving”. These substrates typically lack electrons, so they will be the substrate *being attacked* in the reaction
 - Electrophilic substrates will have + charges
 - A **nucleophile** serves as an electron pair donor and has an extra pair of electrons, which usually *attacks* other electrophilic substrates

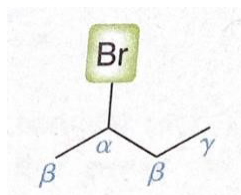


- **What makes a good nucleophile?**

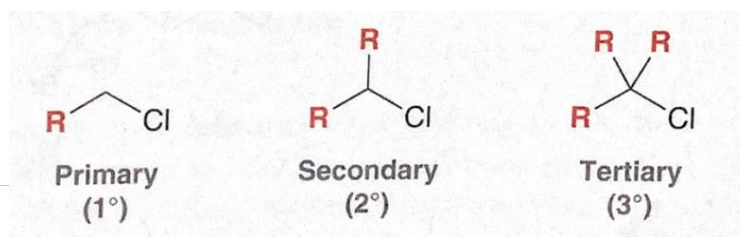
- The greater the negative charge, the more likely an atom will give up its electrons to form a bond! So, the greater the negative charge, the more nucleophilic that species is!
- An anion is always a better nucleophile than a neutral molecule, so the conjugate base is always a better nucleophile
- A highly electronegative atom is a poor nucleophile because it is unwilling to share its electrons.

HIGHLIGHT #1: Structure of Alkyl Halides

- Understanding the structure of alkyl halides is very important when determining whether a reaction will proceed via SN1 or SN2.
- The **alpha position** is the carbon that is directly connected to the halogen, while the **beta position** is the carbon atom connected to the alpha position



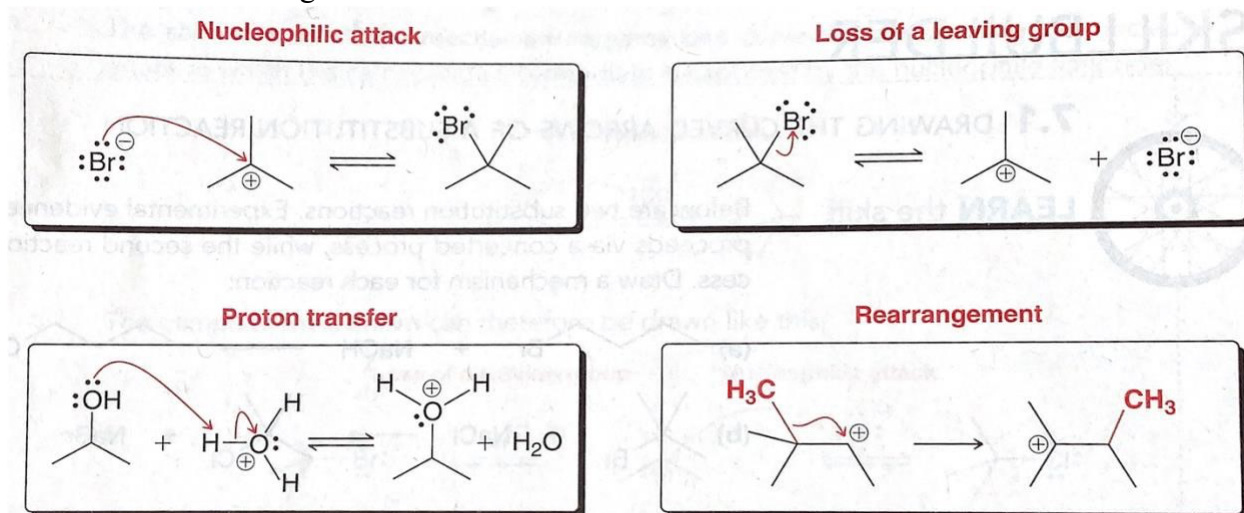
- Alkyl halides are classified by the number of alkyl groups connected to the alpha position



- A primary carbon only has one other R group attached to it
 - A secondary has 2 other R groups attached to it
 - A tertiary group has 3 other R groups attached to it
-

HIGHLIGHT #2: Patterns for Substitution Reactions

1. There are four common patterns to every substitution reaction, however an SN1 and SN2 reaction exhibit different combinations of patterns
2. The four patterns are:
 - Nucleophilic attack
 - Loss of a leaving group
 - Proton transfer
 - Rearrangement



- There are two possible ways a substitution reaction can occur:
 - A *concerted process*: where a nucleophile attacks and the leaving group leaves at the same time
 - A *stepwise process*, where the leaving group leaves first, and then that prompts the nucleophile to attack

Practice #1: Let's assume that your Organic Chemistry professor told you that the first reaction is concerted, and the second reaction is stepwise. Practice drawing out the mechanism for each reaction:

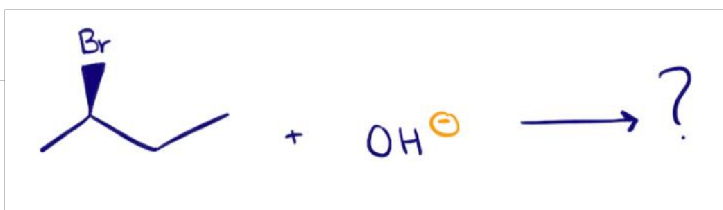


HIGHLIGHT #3: SN2 Mechanism Breakdown

There are a couple of things we need to learn for SN2 mechanisms before we get more practice with learning how to draw mechanisms, such as learning which of the four patterns SN2 mechanisms exhibit.

- An SN2 reaction is a **second order reaction** because it depends on the concentration of two different compounds
- Since the substrate and the nucleophile collide with each other, an SN2 reaction is said to be **bimolecular** because of the two separate entities that interact with each other
- Because of this, SN2 reactions are concerted and involve a *nucleophilic attack* and a *loss of a leaving group* happening at the same time
 - Because this step is happening at the same time, the rate is determined by the concentration of BOTH the nucleophile and the substrate
 - That is why this is a second order reaction!
- Stereospecificity
 - SN2 reactions proceed through a **back-side attack**, which then leads to an inversion of configuration
 - An **inversion of configuration** means that if the reactant was in an R configuration, the product after the SN2 reaction will be in the S configuration
 - That is why **SN2 reactions are said to be stereospecific**, because the configuration of the product is dependent on the configuration of the starting material
- Structure of the substrate
 - SN2 reactions will occur fastest with primary alkyl halides! Secondary alkyl halides react more slowly, and tertiary alkyl halides are unreactive towards SN2
 - If you see a **primary alkyl halide, that is a good indicator that it will proceed SN2!** A secondary alkyl halide can proceed via SN2 or SN1, so it might be necessary to analyze other things, such as nucleophile strength, strength of the leaving group, etc. A tertiary alkyl halide will never proceed SN2.
- Strength of the nucleophile and leaving group
 - Since the nucleophile is attacking while the leaving group is leaving, ***you need a very strong nucleophile! The leaving group does not have to be very good, if the nucleophile is very strong, the reaction will still occur***

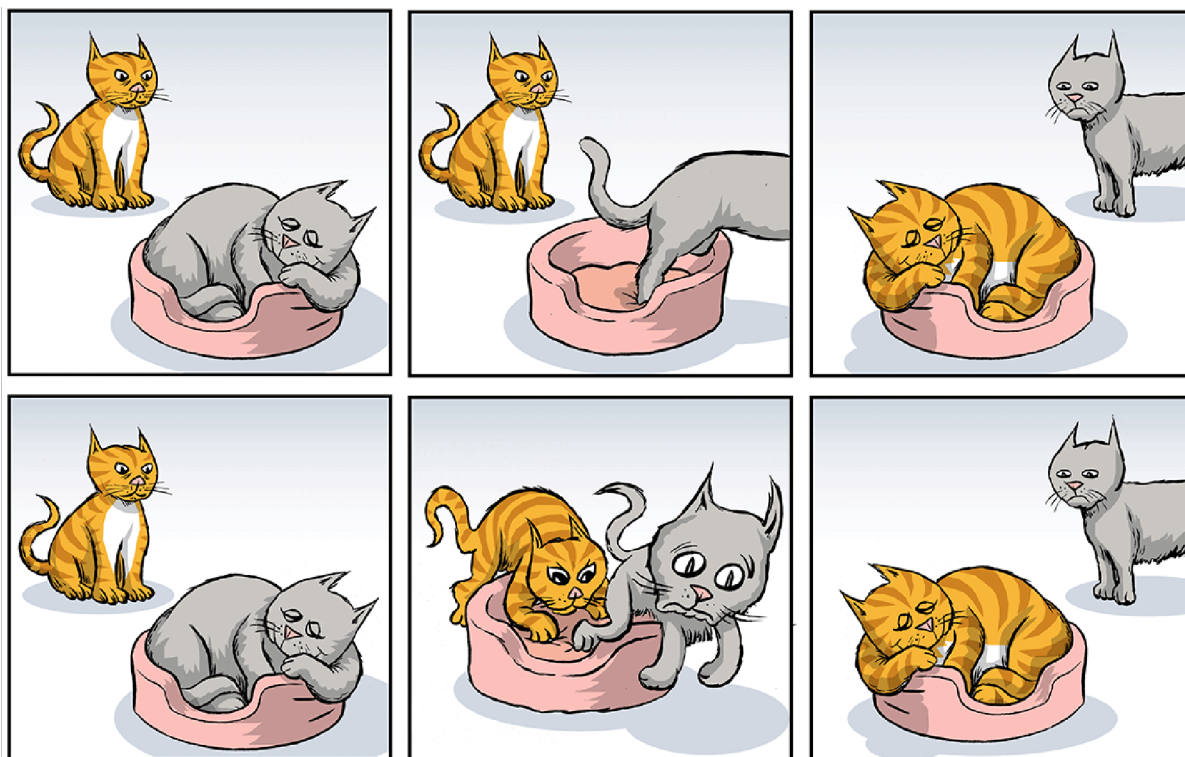
Practice #2: Draw the SN2 product that is obtained for each of the following:



HIGHLIGHT #4: SN1 Mechanism Breakdown

Remember to keep SN2 reactions locked in a different place in your memory file cabinet. They are very different so take some time to make sure you understand their differences!

- An SN1 reaction will NOT follow **second order kinetics, like SN2!**
 - An SN1 reaction is a leaving group leaving which then prompts a nucleophile to attack
 - The rate limiting step in this process is the leaving group leaving. It does not matter how slow or fast the nucleophile is, it will not attack unless the leaving group leaves! That is why **SN1 reactions are unimolecular and first order!** Because the *rate of the reaction is only dependent on the substrate!*
- Because of this, SN1 reactions are stepwise and involve a *loss of a leaving group, followed by a potential carbocation rearrangement, and lastly a nucleophilic attack*
- Stereospecificity ○ We saw that SN2 reactions had an inversion of stereochemistry
 - SN1 mechanisms involve forming a carbocation intermediate, which can then be attacked from either side, leading to BOTH inversion of configuration and retention of configuration!
 - Therefore, **SN1 reactions will produce a racemic mixture** (equal mixture of inversion of stereochemistry and retention of stereochemistry)
- Structure of the substrate ○ **SN1 reactions react most quickly with tertiary substrates!** ○ Primary alkyl halides are mostly unreactive with SN1 mechanisms!
 - For SN2 reactions, we were mainly concerned with steric hindrance, which is why they prefer primary substrates! The nucleophile cannot attack, and the leaving group cannot leave if it is cluttered with steric hindrance.
 - For SN1, we do not have to worry about steric hindrance because our first step does NOT involve a nucleophile attacking!
- Strength of the nucleophile and leaving group ○ Since the leaving group is leaving first, we **MUST HAVE A VERY GOOD LEAVING GROUP! A very strong nucleophile is not necessary! The importance here is on the first step, the loss of a leaving group!**



Practice #3: This is a great picture to emphasize the difference between an SN1 and an SN2!
 Try to guess which row is SN2 and which is SN1!

CHECK YOUR LEARNING:

1.



2.



THINGS YOU MAY STRUGGLE WITH:

- Spend some time making sure you understand the difference between an SN1 and SN2 reaction. Draw out some flashcards and make sure to memorize all the steps involved in both reactions and taking time to ensure you understand their differences.

SUMMARY VIDEOS

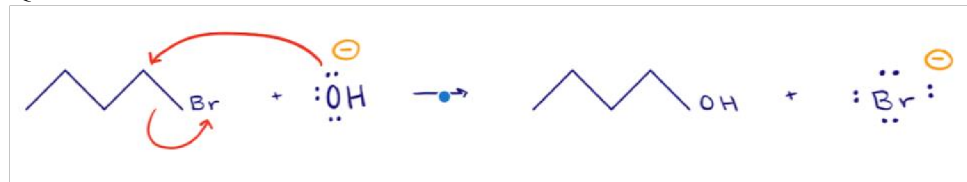
Khan Academy Link: <https://www.youtube.com/watch?v=Z4F88tTx9-8>

Baylor Tutoring Videos: <https://www.youtube.com/watch?v=rzFWWcooMqo>

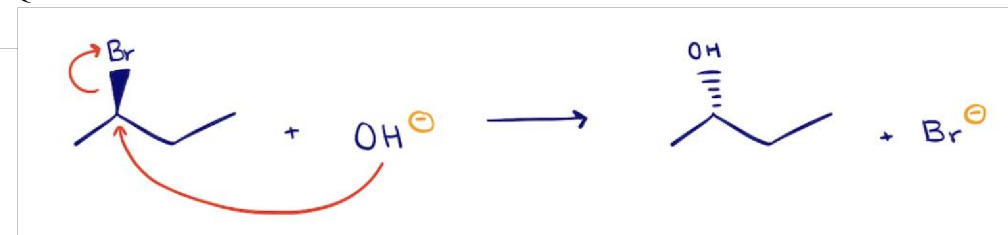
Thanks for checking out these weekly resources!
Don't forget to check out our website for group tutoring times, video tutorials and lots of other resources: www.baylor.edu/tutoring ! Answers to check your learning questions are below!

ANSWERS TO PRACTICES 1-2:

Question 1:



Question 2:



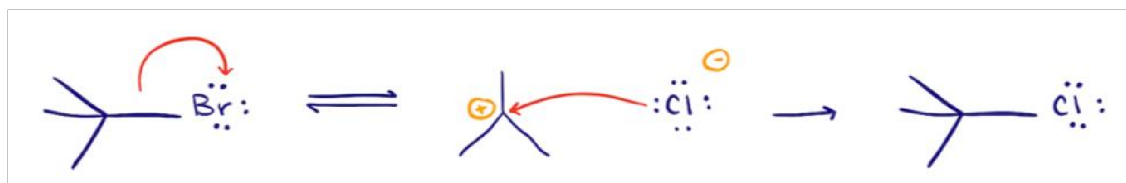
Question 3:

Top row is SN1

Bottom row is SN2

ANSWERS TO CHECK YOUR LEARNING:

Question 1:



Question 2:

