



ScienceGuyz

CHEM 2212

Remembering First Semester Organic Chemistry

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Nomenclature Rules from Organic 1

Basic Nomenclature of Alkanes

- Determine the parent chain of the compound:** The parent chain will be the longest, continual chain of carbons. Note that the longest chain will not always be read from left to right! The name of the longest continual chain of carbons can be determined from the names contained in the chart below:

Number of Carbons in Chain	Name	Number of Carbons in Chain	Name
1	Methane	8	Octane
2	Ethane	9	Nonane
3	Propane	10	Decane
4	Butane	11	Undecane
5	Pentane	12	Dodecane
6	Hexane	13	Tridecane
7	Heptane		

- Number Parent Chain:** Once the parent chain has been determined, number down through the parent chain in whichever direction will give the substituent (branch attached to the parent chain) closest to the end of the chain the lowest locant (number).
- Identify Substituents:** Identify the substituents attached to the parent chain.
 - Alkyl Substituents:**
 - Carbon substituents will be named by determining the longest chain of the substituent.
 - Carbon 1 of the alkyl substituent will ALWAYS be the carbon that is directly attached to the parent chain.
 - Remove the suffix –ane from the name of the substituent and replace it with the suffix –yl.

Example: Methane (1 carbon substituent) → Methyl

- Halogen Substituents:** Halogen substituents will be named by removing the suffix –ine of the halogen and replacing it the suffix –o.

Example: Bromine → Bromo

4. Assemble Name:

- Assemble the name of the compound by alphabetizing the substituents using the first letter in the name of each substituent.
- Each substituent should include a locant which will be placed in front of the substituent name. The locant will serve to identify where on the parent chain the substituent can be found.
- Each locant should be separated from each substituent name with a dash.
- Name the parent chain last. (NEVER INCLUDE A DASH OR A SPACE BETWEEN THE LAST SUBSTITUENT AND THE PARENT CHAIN)

Example: 1-bromo-2-chloro-3-methylhexane

5. When there is more than one substituent of a given type in a structure:

- Aggregate the substituents together into one substituent name.
- Add a prefix (di, tri, tetra, penta, etc....) which indicates how many substituents of that type are present in the compound.
- Indicate the locant at which each identical substituent appears on the parent chain.
- Place each locant in front of the substituent name, in numerical order, separating each locant with a comma.
- Never alphabetize using prefixes such as di, tri tetra etc... unless the substituent has branching (complex substituent).

Example: 1,2,3-trichlorohexane

- If an alkane has more than one longest chain, choose the longest chain that has the greatest number of substituents.

6. Complex Substituents: Complex substituents correspond to substituents which contain branching within a substituent. Complex substituents can be named using systematic naming conventions or using common names.**a. Systematic Nomenclature of Complex Substituents:**

- Find the longest chain in the complex substituent and number it.
- Carbon 1 must ALWAYS correspond to the carbon of the complex substituent which is directly attached to the parent chain.
- Determine the name of the complex substituent's longest chain (REMEMBER TO EXCLUDE ANY CARBONS WHICH ARE IN YOUR PARENT CHAIN). Name the longest chain of the complex substituent replacing the suffix -ane with -yl
- Determine all substituents attached to the longest chain of the complex substituent and their corresponding locants.
- Assemble the name of the complex substituent as you would normally assemble any name (Remember to alphabetize).
- Place the name of the complex substituent in parenthesis and integrate the complex substituent name into the name of the compound, placing the locant of the complex

substituent outside of the parenthesis, as to identify where the complex substituent appears on the parent chain.

- vii. When alphabetizing a complex substituent that you have named using systematic nomenclature conventions, ALWAYS alphabetize the complex substituent's name by the first letter within the parenthesis, regardless of prefixes (Includes prefixes such as di, tri, and tetra).
- b. **Common Names:** Some complex substituents also have common names associated with them. You must memorize the common names of the substituents shown below. When using common names to name an organic compound remember the following:
 - i. Never use parenthesis when using a common name.
 - ii. Never alphabetize with using the prefixes tert- and sec-.
 - iii. Always alphabetize using the prefixes neo- and iso-.
 - iv. The common name iso-: The common name iso- is used when the methyl group at the end of an alkyl substituent is moved inward to the second to last carbon.
- c. **When to Use Common or Systematic:** Unless your professor states otherwise, you can name complex substituents using common names or systematic. However, if you choose to use common names, you must name all substituents which have a common name, by their common name. (No mixing and matching!)

7. Ether Nomenclature (C-O-C compounds): Ethers can be named in two ways:

- a. **Simple Ethers:**
 - i. Name each alkyl group attached to both sides of the oxygen making the ether, in alphabetical order.
 - ii. The name of the compound will end with the name *ether*.
 - iii. Simple ethers correspond to ethers which either have no branching in their alkyl groups or ethers which have branching in their alkyl groups but have associated common names.
- b. **Complex ethers (most commonly used in nomenclature, can be used all of the time)**
 - i. Determine parent chain and identify the ether which is attached.
 - ii. Determine the name of the non-parent alkyl group that is attached to the oxygen.
 - iii. Replace the "yl" with of the alkyl chain name with the suffix "oxy".
 - iv. Integrate this substituent into the name like any other substituent, using a locant.

Example: Methane (1 carbon substituent) → Methoxy

- 8. Nomenclature of Cycloalkanes:** First determine if the cycloalkane is a parent or a substituent:
- Parent cycloalkanes will usually have the functional group which is highest in priority attached to the cyclic ring.
 - If there is no substituent which has highest priority, the ring will act as the parent if it has more carbons than any single substituent attached to the cyclic ring.
 - If the cyclic ring is the parent, number around the cycloalkane, always giving locants one and two to the carbons in the cyclic ring which, in turn, gives all other substituents the lowest possible locant. (Carbon 1 of a substituted cyclic ring must ALWAYS bear a substituent)
 - Alcohols and amines will take **PRIORITY** and are given the lowest locant regardless of whether numbering in another way will provide other substituents a lower locant.
 - If you can number in any direction and still give the substituents the lowest locants, give the substituent which falls closer to "A" on the alphabet the lowest locant.
 - The parent chain of the cycloalkane will be named by placing the prefix "cyclo-" in front of the alkane name.
 - If there is a cycloalkane substituent, name the cycloalkane and remove the suffix -ane and replace it with -yl.
 - Assemble the name as you would any other compound.
 - Stereochemistry in Cycloalkanes:** When a cycloalkane has EXACTLY two substituents attached to it and the two substituents have wedges or dashes, the cycloalkane is said to have stereochemistry.
 - Cis: The two substituents attached to the ring are pointed in the same direction.
 - Trans: The two substituents attached to the ring are pointing in opposite directions.
 - Integrating Stereochemistry into a Name:** Name the compound and place the stereochemistry in front of the entire name. The stereochemistry should be placed inside parenthesis and should be separated from the name with a dash.

- 9. Nomenclature of Priority Groups:** When other functional groups such as alcohols, amines, alkenes or alkynes are present, there may be a priority issue to consider when naming the compound.
- When a functional group of higher priority is present, find the longest chain which includes the highest priority functional group.
 - Even if a longer chain is present, a shorter chain must be chosen if the shorter chain includes the functional group with priority and the longer chain does not.
 - Number down through the longest chain starting at the end of the chain that gives the functional group of highest priority the lowest locant.

Priority Ranking	Functional Group	Parent Chain Name	Substituent Name
1	Alcohol	-ol	n/a
2	Amine	-amine	-amino
3	Alkenes & Alkynes	-ene & -yne	n/a
LAST	Halogens, ethers, alkyl substituents, etc.	n/a	variable

- 10. Alcohol Nomenclature:** The rules for naming alcohols are similar to those of alkanes. However, alcohols will take priority over all functional groups until Organic II.
- Find the longest continual chain of carbons which includes the –OH as a substituent.
 - Number down through the parent chain, starting at the end of the chain which gives the alcohol the lowest locant.
 - To name a parent chain which has only one alcohol, remove the suffix “e” of the alkane parent name and replace it with the suffix “ol”
 - To name a parent chain which has two or more alcohols, leave the suffix “e” of the alkane name and add a prefix designating the number of alcohols present in the compound (di, tri, tetra, etc...) and add the suffix –ol to the parent chain’s name.
 - Designate where the alcohol functional group(s) falls on the parent chain, using a locant which will be inserted, between dashes before the suffix –ol.

Example: Hexane → Hexan-1-ol

- If multiple alcohols are present insert all alcohol locants between the parent and the suffix, in numerical order, separating each with commas.

Example: Hexane → Hexane-1,2,3-triol

11. Amine Nomenclature: The rules for naming amines are similar to those of alcohols and alkanes. However, amines will take priority over all functional groups except alcohols.

- Determine the longest continual chain of carbons which includes the –N as a substituent. (unless an alcohol is present)
- Number down through the parent chain starting at the end of the chain which gives the amine the lowest locant. (unless an alcohol is present)
- To name a parent chain which has only one amine, remove the suffix “e” of the alkane parent name and replace it with the suffix “amine”
- To name a parent chain which has two or more amines, leave the suffix “e” of the parent name and add a prefix designating the number of amines present in the compound (di, tri, tetra etc...) and add the suffix –amine to the parent chain’s name.
- Designate where the amine functional group(s) fall on the parent chain using a locant which will be inserted, between dashes before the suffix amine.

Example: Hexane → Hexan-1-amine

- If multiple amines are present, insert all amine locants between the parent and the suffix in numerical order, separated by commas.

Example: Hexane → Hexane-1,2,3-triamine

- If alkyl substituents are present on the nitrogen of the amine, integrate them into the name of the compound as you would any other substituent. These substituents will have the locant “N”.
- If an alcohol and an amine are on a compound, the alcohol will take priority, and the amine will be named as an *amino* substituent.

12. Nomenclature of the Alkene & the Alkyne

- Use the standard nomenclature rules, however double bonds & triple bonds will take priority. Number down the parent chain giving the double bonds or triple bonds the lowest locant possible (except when alcohols or amines are present)!
- Between alkenes and alkynes, the multiple bond which is closer to the end of the chain will take priority; otherwise, the alkene will take priority.
- The suffix for alkenes will be –ene.
- The suffix for alkynes will be -yne.
- No matter what, always list the alkyne after the alkene in the name.
- Each double bond/triple bond will be identified in the name using the locant in which the double bond/triple bond begins.
- More than one double bond will be named as a diene, triene, etc...
 - Or diyne, triyne, etc...

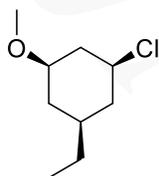
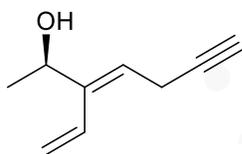
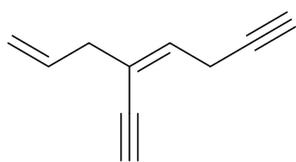
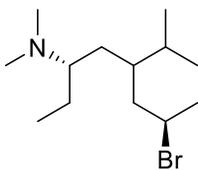
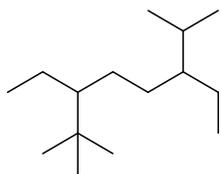
13. Identifying and Integrating R/S Stereochemistry

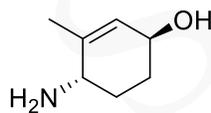
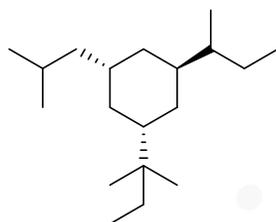
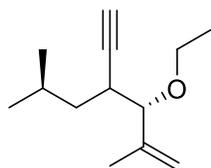
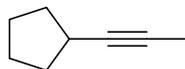
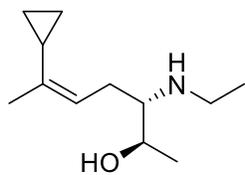
- a. Remember that a chiral center is an atom that is bound to four different substituents.
- b. Chiral centers can have either R or S stereochemistry.
- c. To determine if a chiral center is R/S:
 - a. Identify the chiral center.
 - b. Assign priority to substituents by working outwards, atom by atom, from the chiral center. The higher the atomic mass, the higher the priority.
 - c. Ensure the lowest priority is on the back (dashed). If it is not, switch it with whatever group is on the dash.
 - d. Draw directionality arrows from $1 \rightarrow 2 \rightarrow 3$.
 - i. **R stereochemistry:** If the arrows move clockwise.
 - ii. **S stereochemistry:** If the arrows move counterclockwise.
 - iii. Note: if you had to switch the lowest priority to the back, the stereochemistry of the original compound will be opposite of the stereochemistry determine for the switched compound.
- d. To integrate this stereochemistry into the name, place in front of the name in parenthesis.
- e. If there is only one chiral center, DO NOT use a locant to identify the stereochemistry. If there are multiple chiral centers, a locant is necessary.

14. Identifying and Integrating E/Z Stereochemistry

- a. Remember that a double bond will have stereochemistry if there are two different substituents attached to the sp^2 hybridized carbons of an alkene.
- b. Double bonds can have either E or Z stereochemistry.
- c. **To determine if a double bond is E/Z:**
 - a. Identify the double bond with stereochemistry.
 - b. Draw a dotted line perpendicular to the double bond, thru the middle of the double bond.
 - c. Look to the left of the line and of the two substituents attached to the sp^2 hybridized carbon, circle the substituent which has highest priority.
 - d. Look to the right of the line and of the two substituents attached to the sp^2 hybridized carbon, circle the substituent which has highest priority.
 - i. **E Stereochemistry:** The two highest priority substituents are pointed in the opposite directions about the double bond.
 - ii. **Z Stereochemistry:** The two highest priority substituents are pointed in the same direction about the double bond.
- d. To integrate this stereochemistry into the name, place in front of the name in parenthesis.
- e. If there is only one double bond with stereochemistry, DO NOT use a locant to identify the stereochemistry. If there are multiple double bonds with E/Z, a locant is necessary.
- f. For cyclic rings which have fewer than 8 members, you will NEVER use E/Z stereochemistry for double bonds.

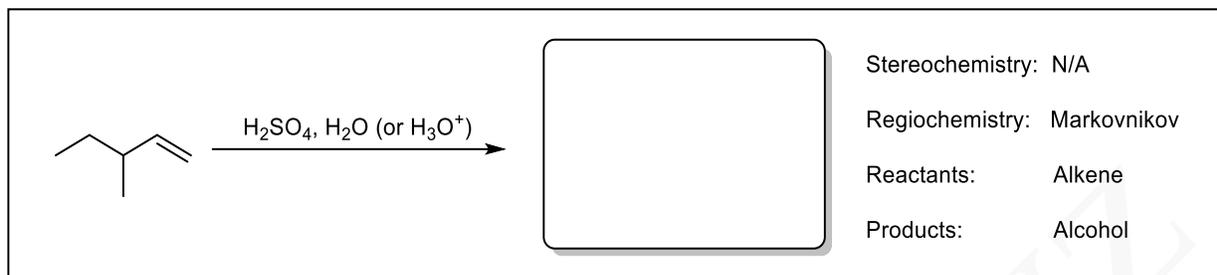
Example: Provide the IUPAC name for each of the following compounds.





Chapter 6: Electrophilic Addition Reactions of Alkenes

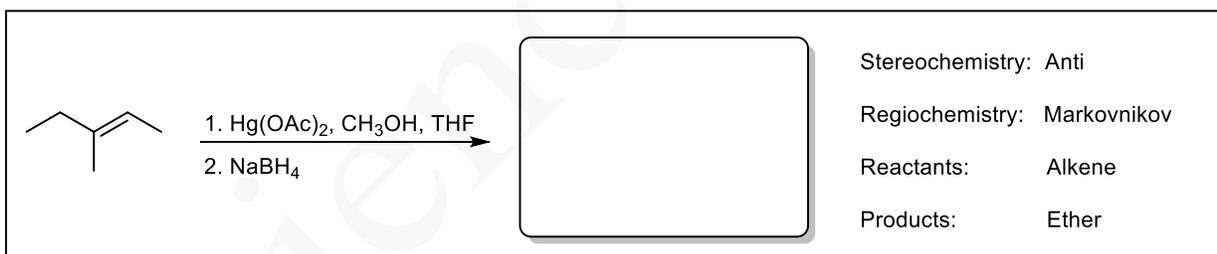
Acid Catalyzed Hydration (Rearrangement Possible)



Oxymercuration/Demercuration

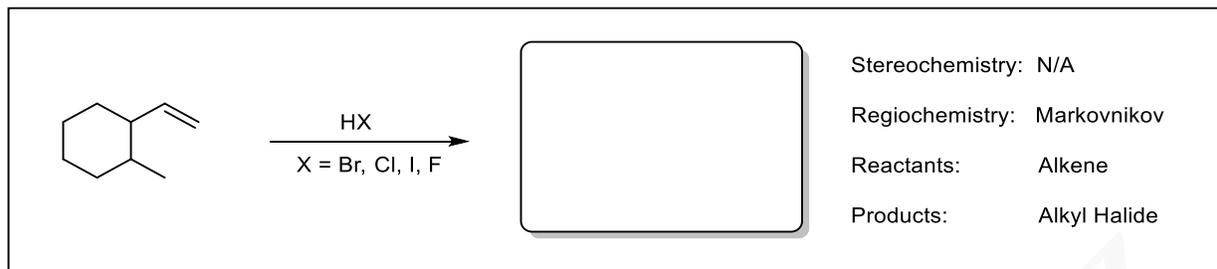
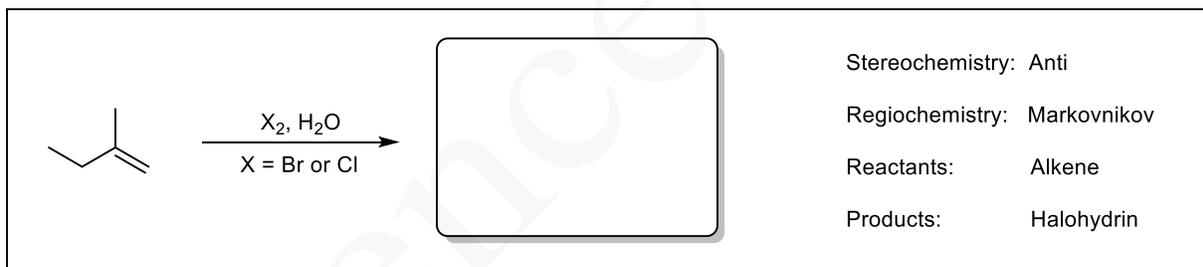
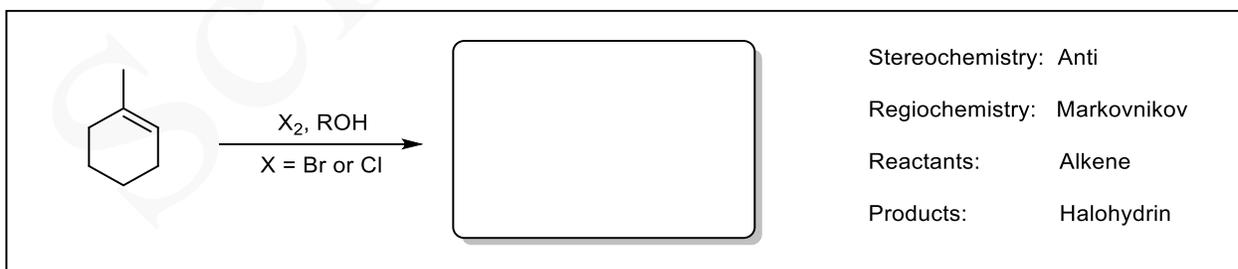


Modified Oxymercuration/Demercuration

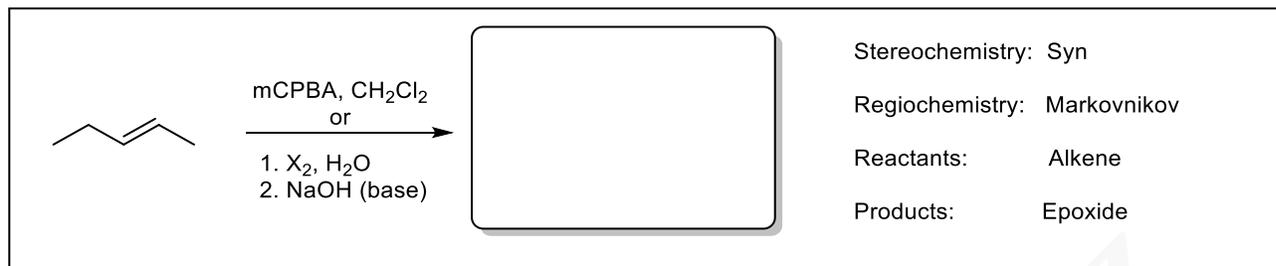


Hydroboration/Oxidation

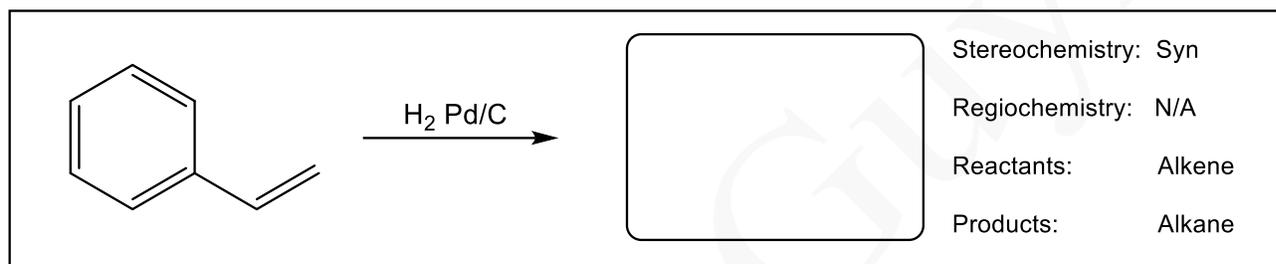


Hydrohalogenation (Rearrangement Possible)**Halogenation****Halohydrin****Modified Halohydrin**

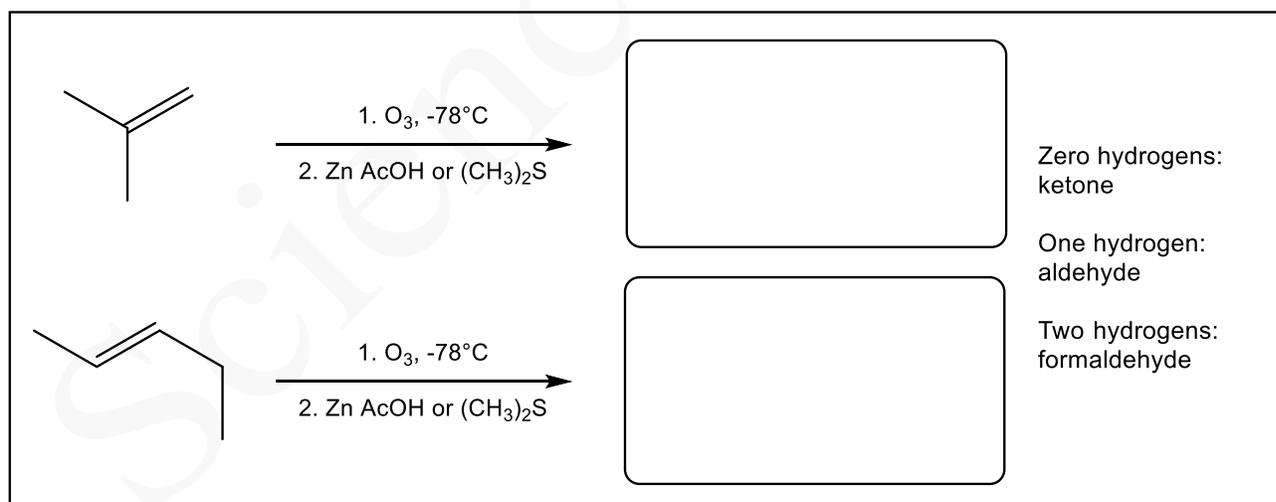
Peroxyacid Epoxidation



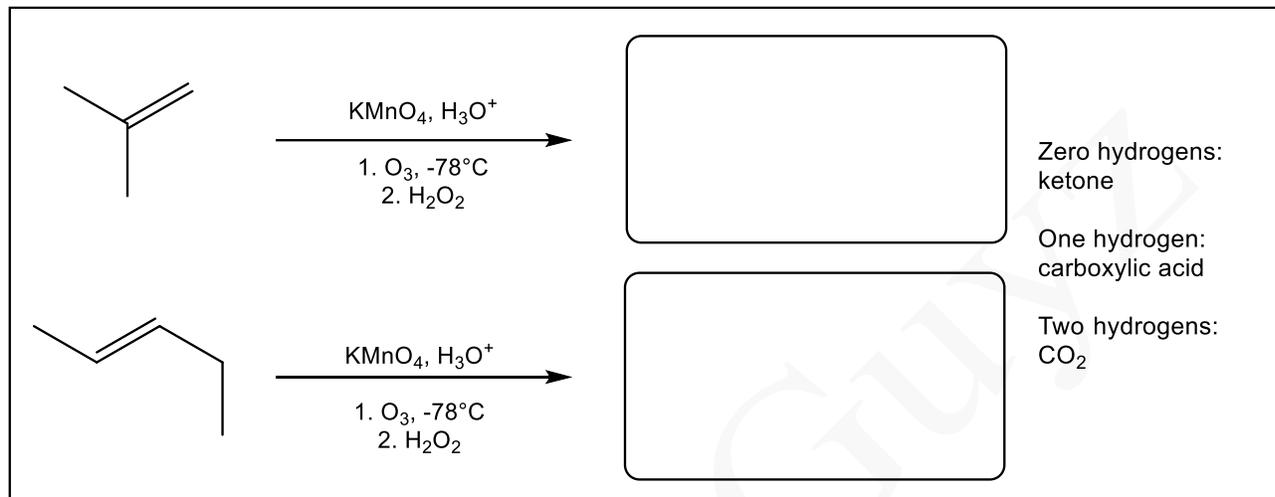
Catalytic Hydrogenation (does not reduce arene double bonds)



Ozonolysis (Reductive Workup): The alkene will cleave down the middle. To determine what products will form, you must see how many hydrogen atoms are attached to the opposing ends of the alkene. Ozonolysis will consume all double bonds in a compound unless they are a part of an arene.

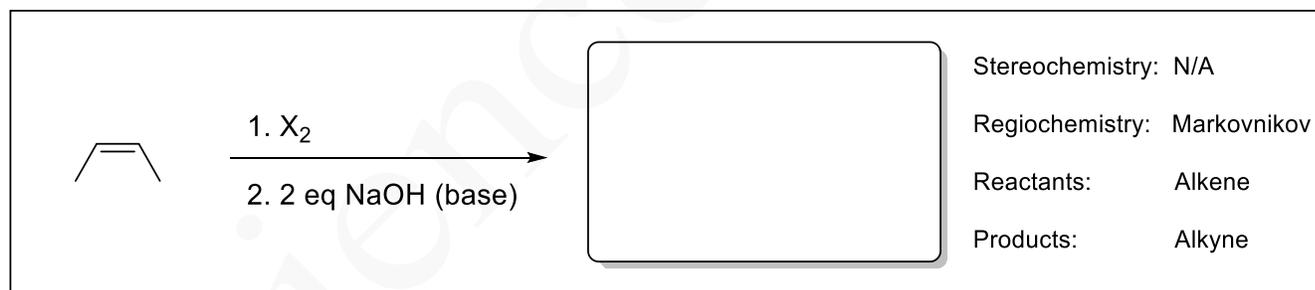


Ozonolysis (Oxidative Workup)/KMnO₄ Oxidation: The alkene will cleave down the middle. To determine what products will form, you must see how many hydrogen atoms are attached to the opposing ends of the alkene. KMnO₄ Oxidation will consume all double bonds in a compound unless they are a part of an arene.

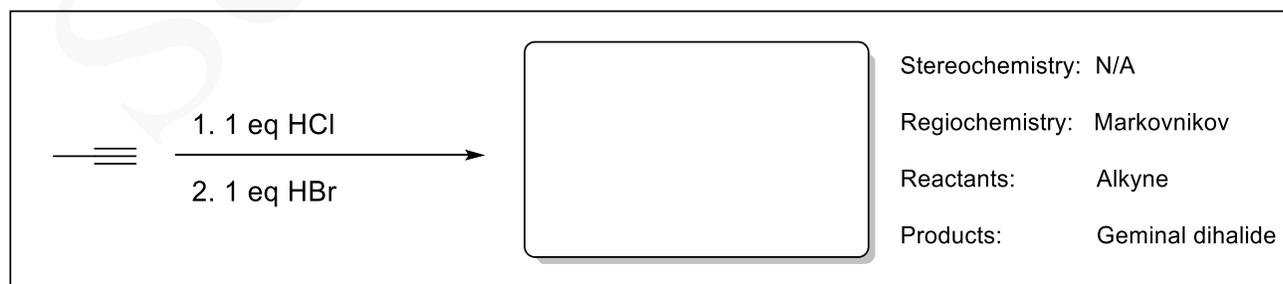


Chapter 7: Reactions of Alkynes

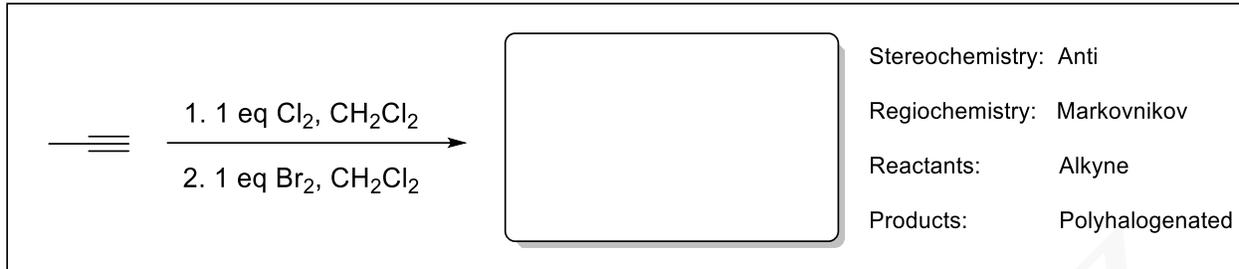
Formation of the Alkyne from the Alkene



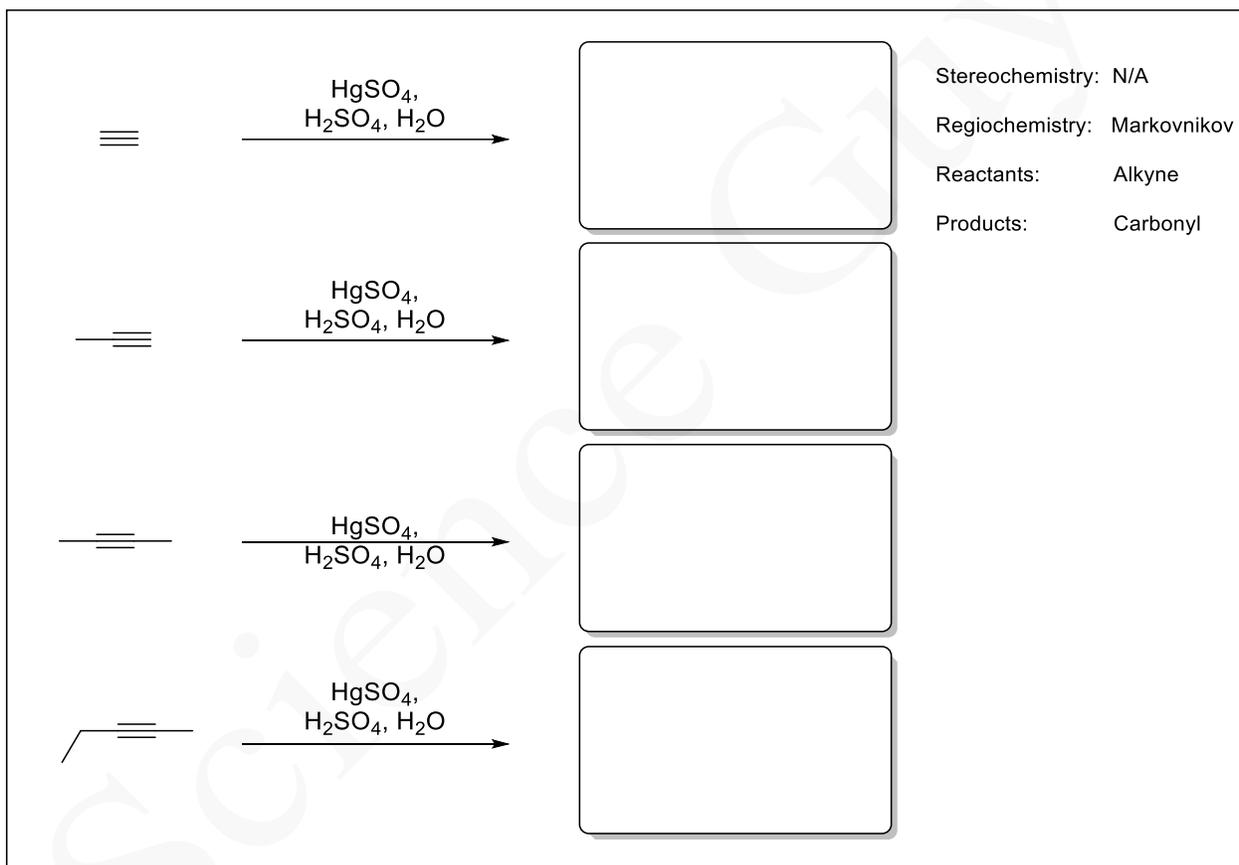
Hydrohalogenation of the Alkyne



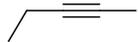
Halogenation of the Alkyne



Mercury Catalyzed Hydration of the Alkyne:



Hydroboration Oxidation of the Alkyne

	$\xrightarrow[2. \text{H}_2\text{O}_2, \text{NaOH}, \text{H}_2\text{O}]{1. \text{9-BBN, THF}}$	<input type="text"/>	Stereochemistry: N/A Regiochemistry: Anti-Markovnikov Reactants: Alkyne Products: Carbonyl Notes: Terminal alkynes must use 9-BBN
	$\xrightarrow[2. \text{H}_2\text{O}_2, \text{NaOH}, \text{H}_2\text{O}]{1. \text{9-BBN, THF}}$	<input type="text"/>	
	$\xrightarrow[2. \text{H}_2\text{O}_2, \text{NaOH}, \text{H}_2\text{O}]{1. \text{9-BBN or BH}_3, \text{THF}}$	<input type="text"/>	
	$\xrightarrow[2. \text{H}_2\text{O}_2, \text{NaOH}, \text{H}_2\text{O}]{1. \text{9-BBN or BH}_3, \text{THF}}$	<input type="text"/>	

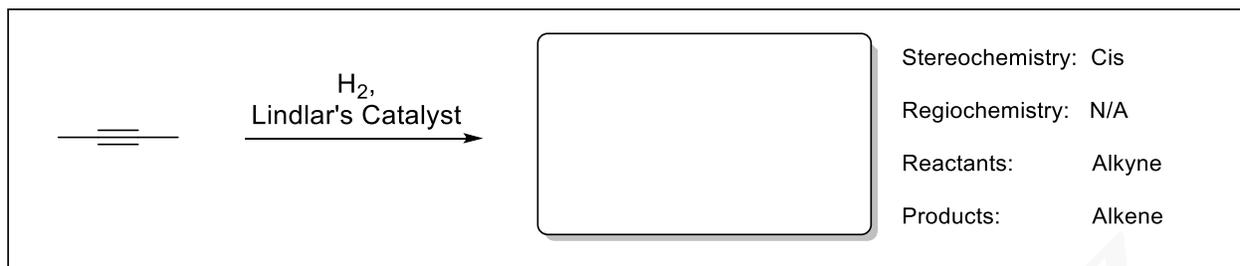
Catalytic Hydrogenation of Alkynes

	$\xrightarrow{\text{H}_2, \text{Pd/C}}$	<input type="text"/>	Stereochemistry: Syn Regiochemistry: N/A Reactants: Alkyne Products: Alkane
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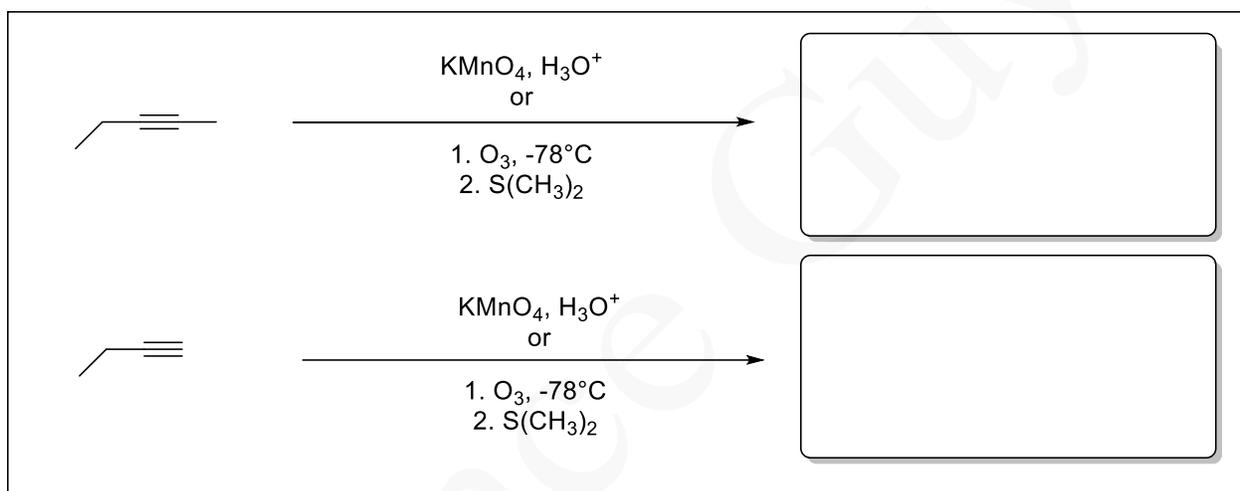
Dissolving Metal Reduction: Produces the trans-alkene. Can NOT be used on terminal alkynes.

	$\xrightarrow[\text{NH}_3, -78^\circ\text{C}]{\text{Na or Li,}}$	<input type="text"/>	Stereochemistry: Trans Regiochemistry: N/A Reactants: Alkyne Products: Alkene
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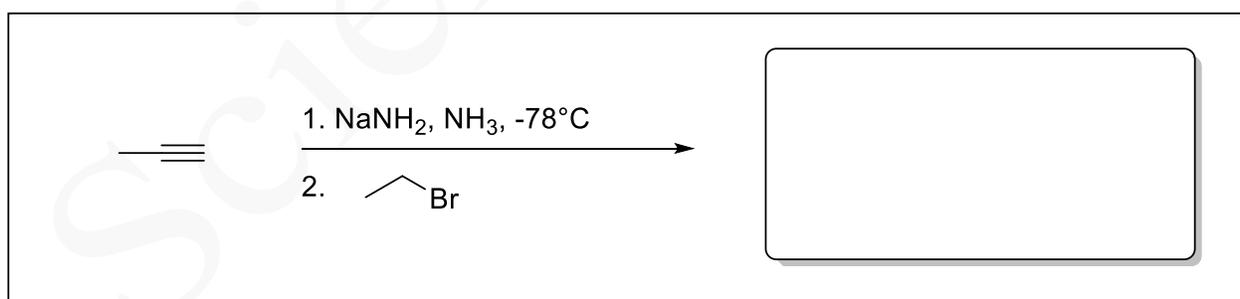
Lindlar's Reduction: Produces the cis-alkene.



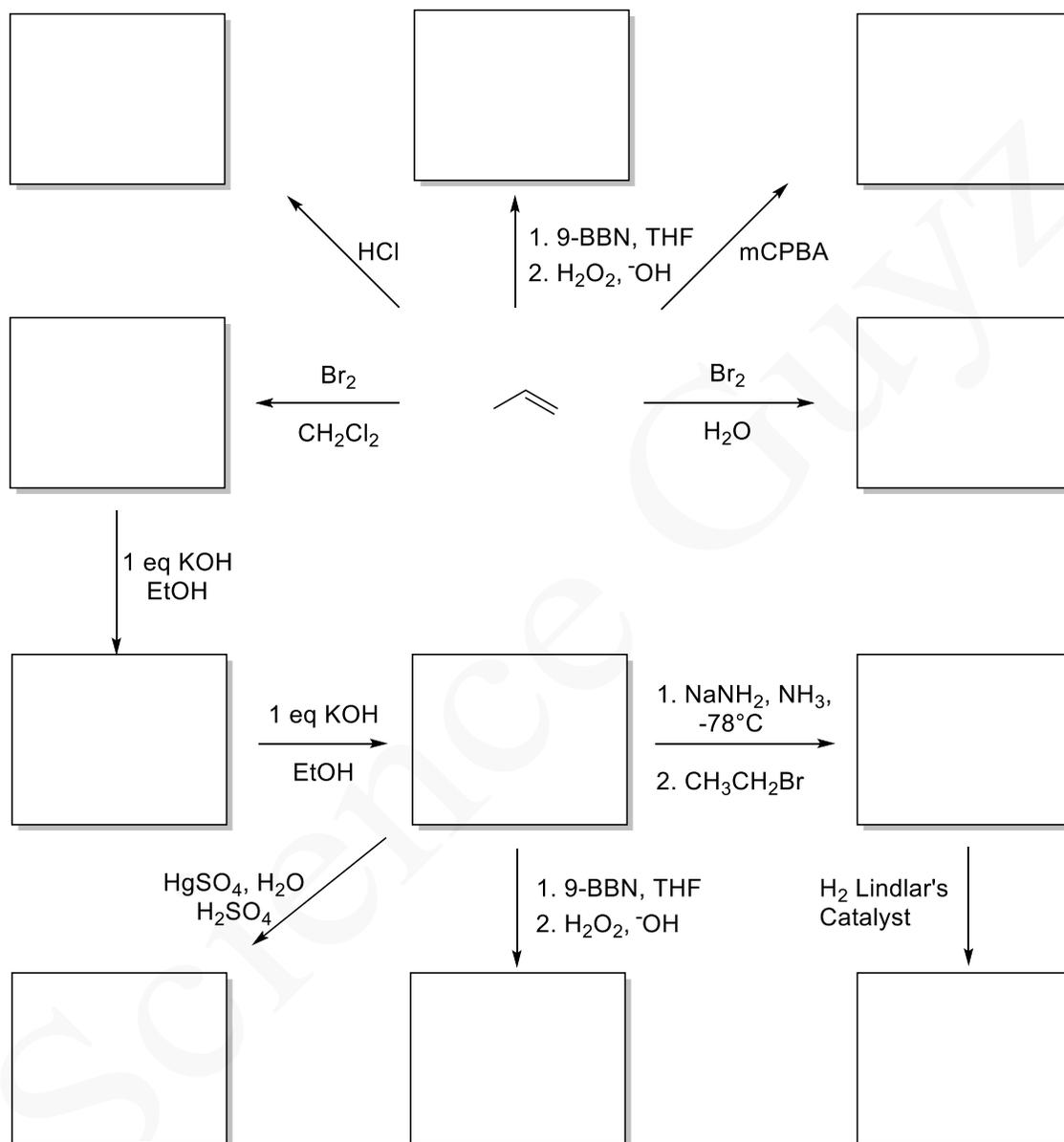
Oxidative Cleavage of the Alkyne: Will always cleave down through the triple bond to produce a carboxylic acid (no terminal Hydrogen) or CO₂ (1 terminal hydrogen).



Alkylation of the Acetylide Anion

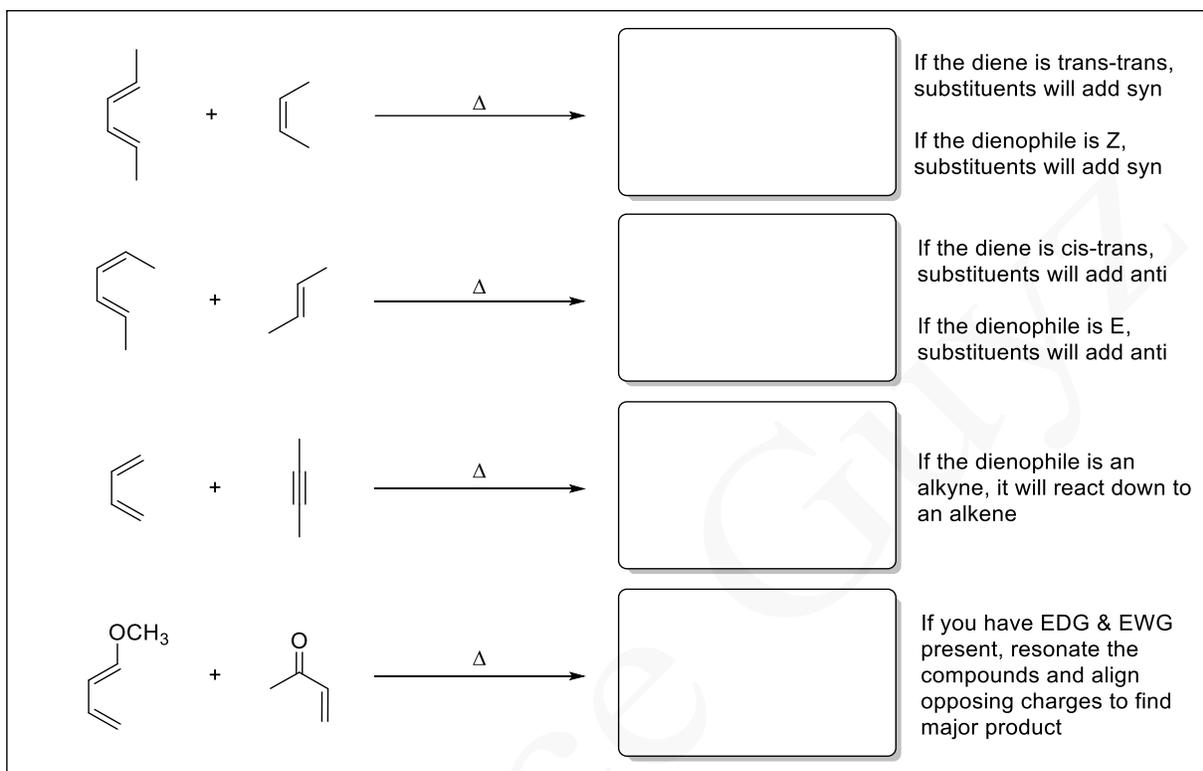


Example: Complete the following spiderweb of reactions by providing the product(s) for each of the indicated reactions.

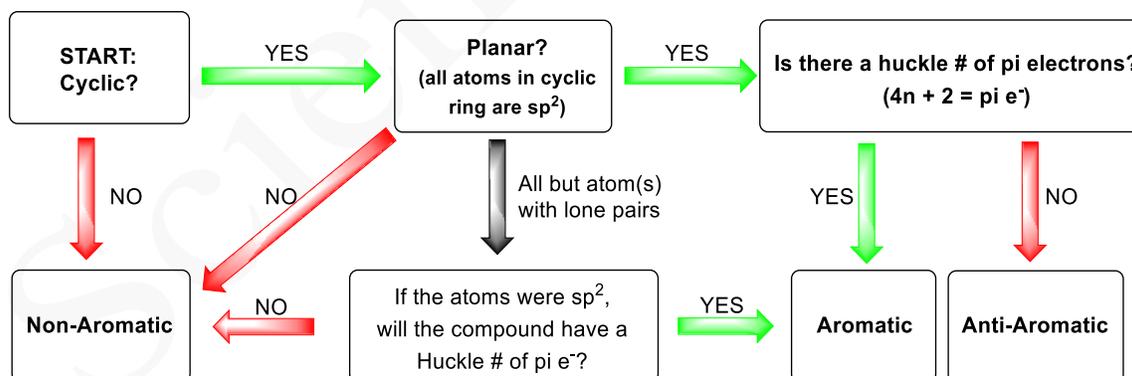


Chapter 8: Conjugation and Aromaticity

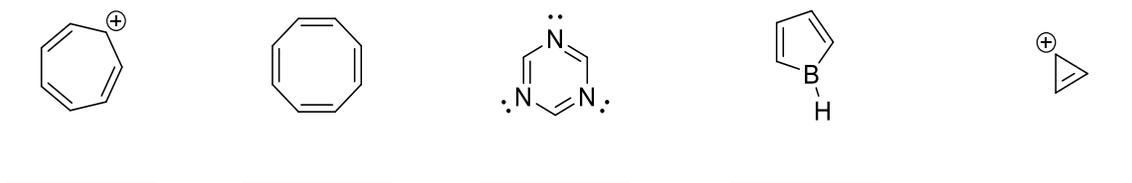
Diels Alder Cycloaddition



Aromaticity

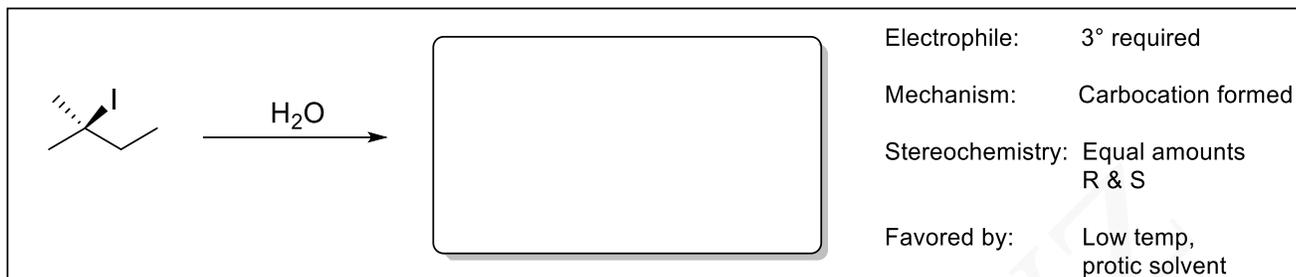


Example: Determine whether the compounds below are aromatic, anti-aromatic or non-aromatic.



Chapter 9: Nucleophilic Substitution and Elimination

S_N1 Reaction (Rearrangement possible)



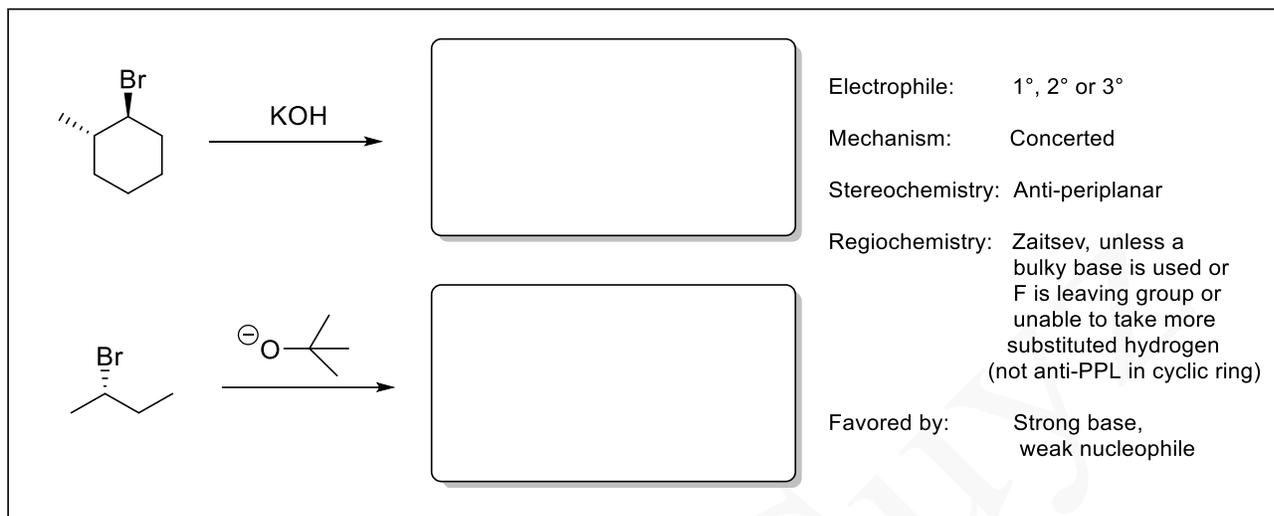
S_N2 Reaction



E1 Reaction (Rearrangement possible)



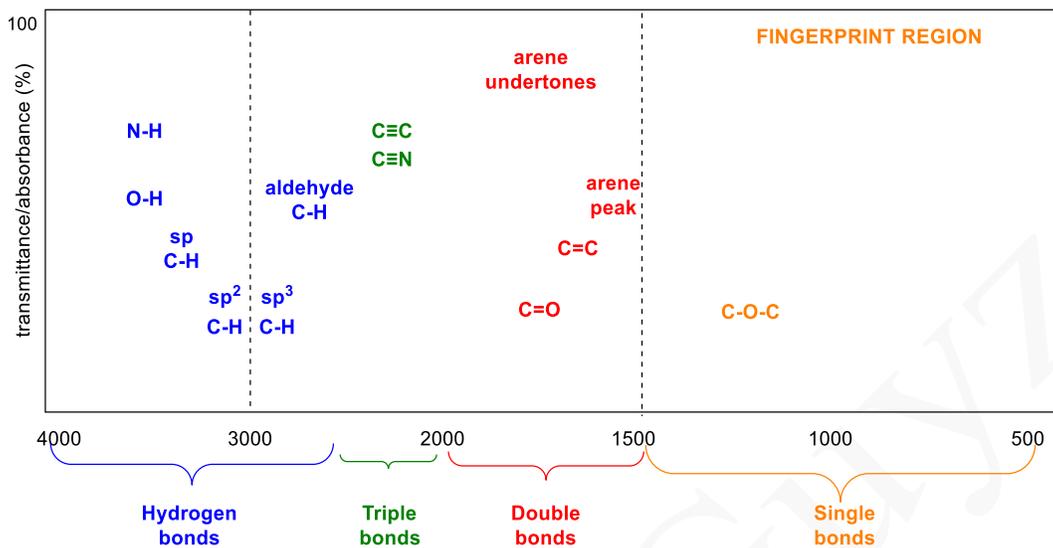
E2 Reaction



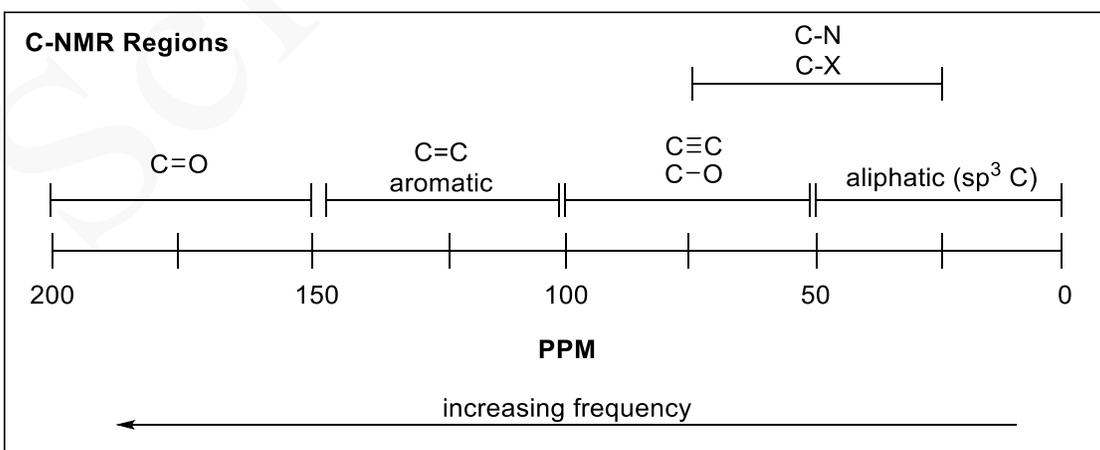
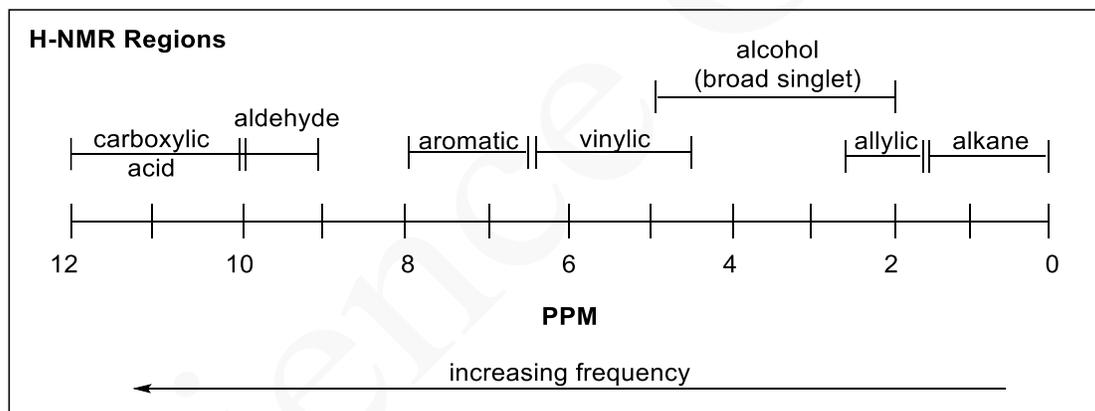
Picking Major Pathway Chart

	Strong Nucleophile/ Strong Base	Weak Nucleophile/ Strong Base	Strong Nucleophile/ Weak Base	Weak Nucleophile/ Weak Base				
	NaOH NaOR	LiCH ₂ CH ₃ NaH	KOC(CH ₃) ₃ DBU	LDA DBN	KCN LiN ₃	NaSR KOOCR	H ₂ O NH ₃	HOCH ₃ HSCH ₃
1° Alkyl Halide	S _N 2	E2 (Δ)	S _N 2	S _N 2	S _N 2 (If nucleophile strength is greater than the fluoride ion; if not, no reaction)			
2° Alkyl Halide	E2	E2	S _N 2	S _N 2 (If nucleophile strength is greater than the fluoride ion) or E1 (Δ)				
3° Alkyl Halide	E2	E2	S _N 1 &/or E1 (Δ)	S _N 1 &/or E1 (Δ)				

Chapter 13: Infrared Spectroscopy

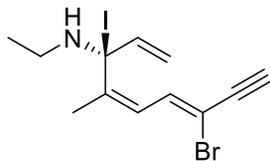
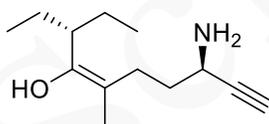
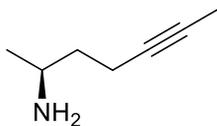
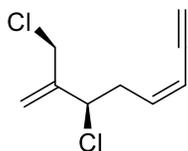
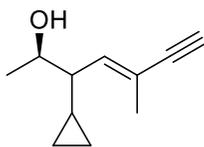
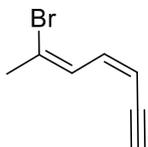


Chapter 14: Nuclear Magnetic Resonance

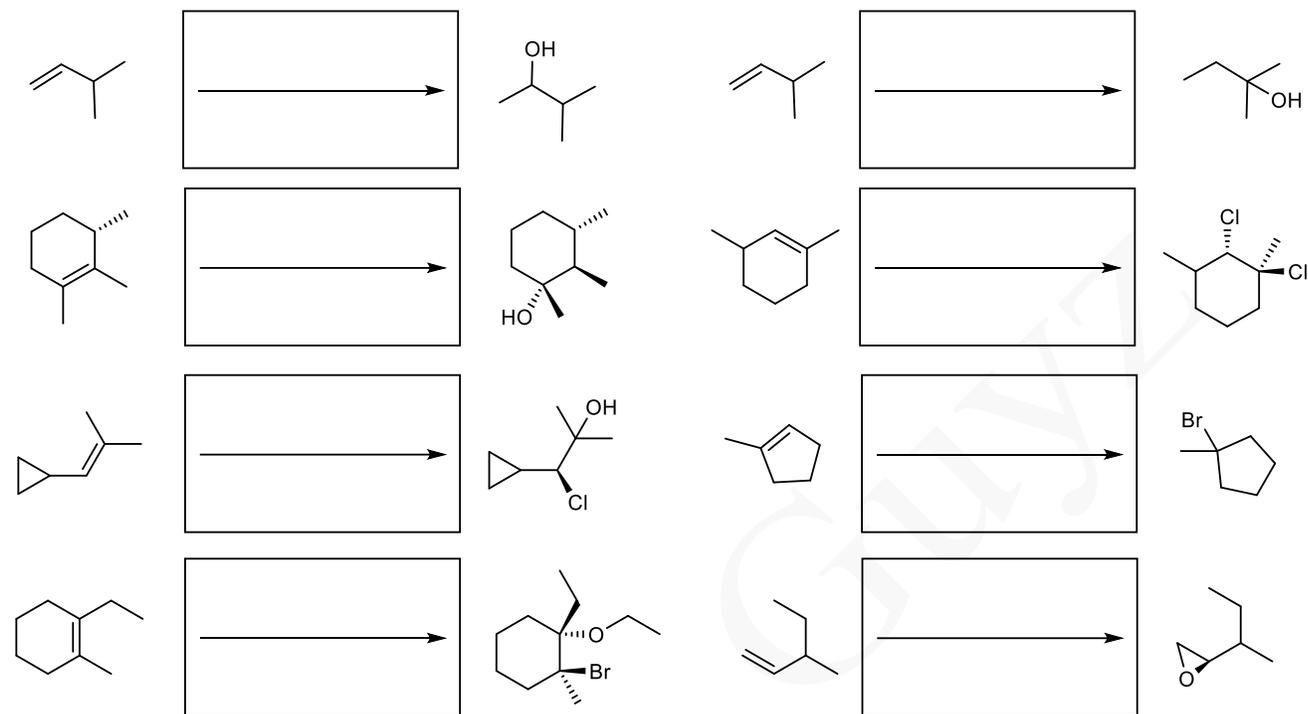


Practice Problems – test your understanding and try these problems out on your own! An answer key will be posted to the Science Guyz website.

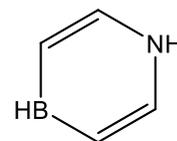
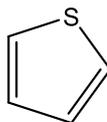
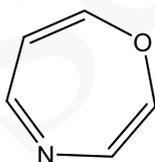
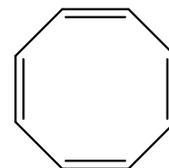
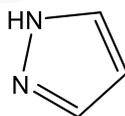
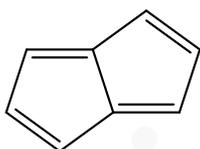
1. Provide the IUPAC name for each of the following compounds.



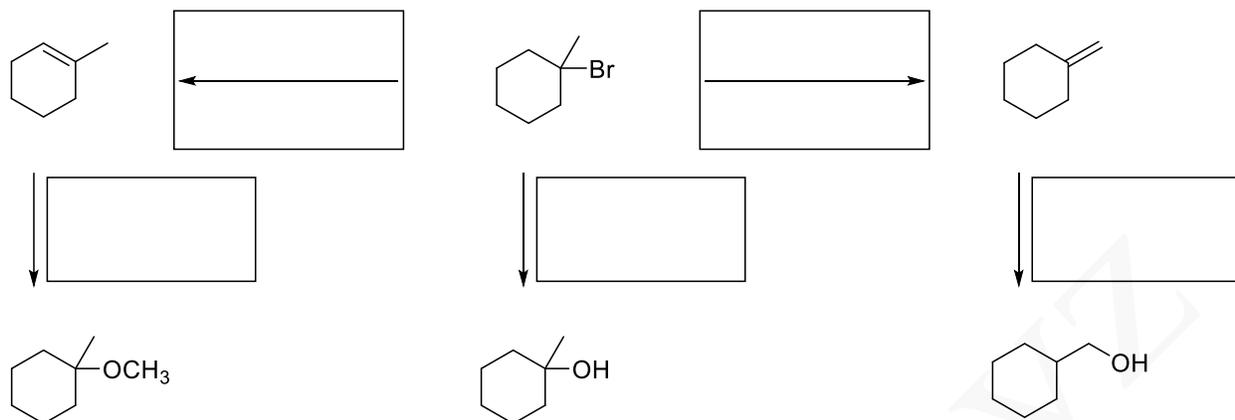
2. Provide the missing reagent(s) for the following transformations.



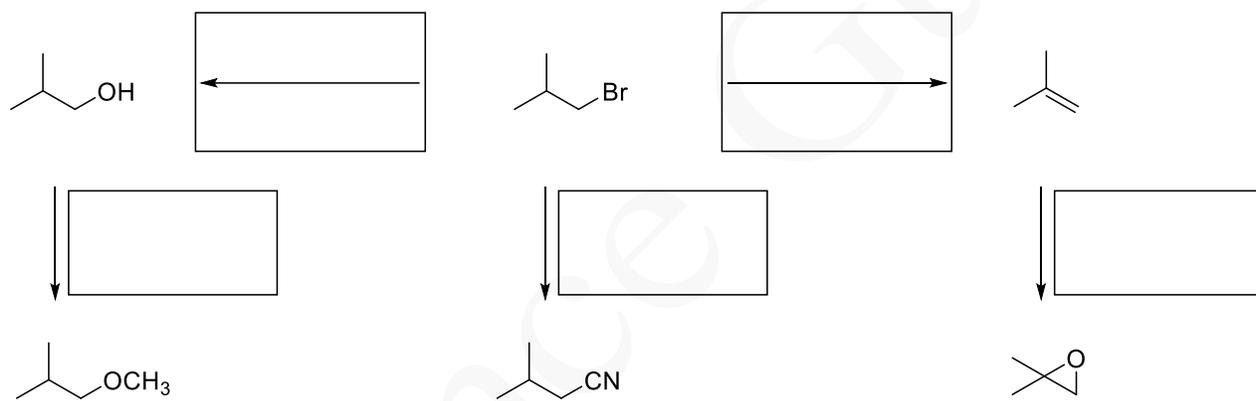
3. Classify each compound as aromatic, antiaromatic, or nonaromatic.



4. Provide the missing reagent(s) for the reactions shown below.



5. Provide the missing reagent(s) for the reactions shown below.



6. Propose a synthesis for the following transformation.

