Presented by: Dr. Baira Fayçal

Fundamentals Of Organic Chemistry

Lessons, Exercises, And Solutions

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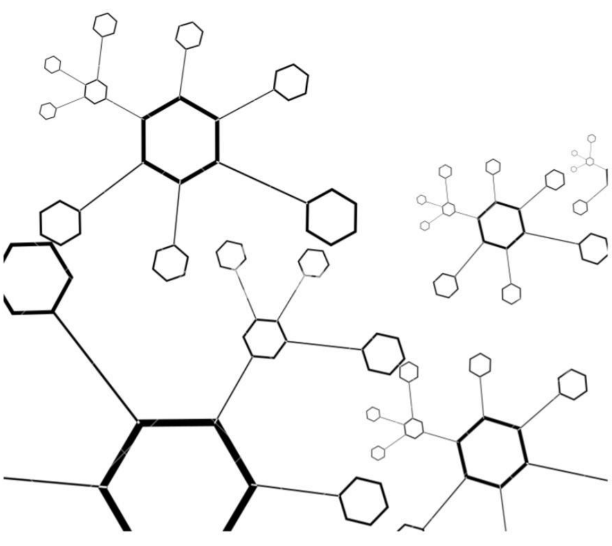
Fundamentals of Organic Chemistry.

Lessons, Exercises, and Solutions

Author:

Dr. Baira Fayçal



Fundamentals of Organic Chemistry.
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E.mail: tohfapublishhouse@gmail.com

Fundamentals of Organic Chemistry

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Preface

Welcome to the world of organic chemistry, a fascinating and dynamic field that lies at the heart of modern science. This educational handout, titled "Fundamentals of Organic Chemistry," is designed to serve as a comprehensive guide for students embarking on their journey through the intricate and captivating realm of organic chemistry. It is with great enthusiasm that I present this material to you, hoping to spark your curiosity and deepen your understanding of this essential branch of chemistry.

Organic chemistry is not just a subject; it is a way of thinking, a framework for understanding the complex interactions of carbon-based compounds that are the building blocks of life. From the simplest hydrocarbons to the most complex biological molecules, the principles of organic chemistry underpin a vast array of scientific disciplines and practical applications. Whether you are pursuing a career in medicine, pharmaceuticals, materials science, or any other field that relies on a deep understanding of molecular interactions, a solid foundation in organic chemistry is indispensable.

This handout is structured to provide a clear and systematic introduction to the fundamental concepts and principles of organic chemistry. It begins with an exploration of the basic structure and bonding in organic molecules, delving into the nature of covalent bonds, hybridization, and resonance. The importance of functional groups is emphasized, as these groups determine the chemical properties and reactivity of organic compounds. The section on nomenclature is crucial for mastering the language of organic chemistry, enabling you to accurately describe and communicate about the vast array of organic molecules.

The study of isomerism and stereochemistry reveals the three-dimensional nature of organic molecules and the profound impact that spatial arrangement can have on their properties and reactions. Understanding acids and bases in organic chemistry is fundamental to predicting and controlling the outcomes of many organic reactions. The subsequent chapters on organic reactions and mechanisms provide a detailed look at the various types of reactions that organic compounds can undergo, including substitution, addition, elimination, and rearrangement reactions. The mechanisms behind these reactions are meticulously explained, helping you to visualize the step-by-step processes involved.

The latter part of the handout focuses on specific classes of organic compounds, such as alkanes, cycloalkanes, alkenes, alkynes, aromatic compounds, alcohols, phenols, ethers, aldehydes, ketones, carboxylic acids, derivatives, amines, and amides. Each class of compounds is examined in detail, with an emphasis on their structures, properties, and characteristic reactions. This in-depth exploration will equip you with the knowledge and skills needed to tackle complex problems and engage in advanced studies in organic chemistry.

Throughout this handout, you will find numerous examples, illustrations, and exercises designed to reinforce your understanding and enhance your problem-solving abilities. The references listed at the end of the handout are invaluable resources for further reading and exploration. They represent a selection of the most respected and comprehensive texts in the field of organic chemistry, providing a wealth of additional information and insights.

As you navigate through this handout, I encourage you to approach each topic with an open mind and a spirit of inquiry. Organic chemistry can be challenging, but it is also incredibly rewarding. The more you engage with the material, the more you will appreciate the beauty and elegance of the subject. I hope that this handout will serve as a valuable companion on your journey, helping you to build a strong foundation in organic chemistry and inspiring you to explore the many exciting opportunities that this field has to offer.

Thank you for choosing to explore the fundamentals of organic chemistry with this handout. I wish you a stimulating and successful learning experience.

Fayçal BAIRA

Chapter 1: Introduction to Organic Chemistry

1.1 What is Organic Chemistry?

Organic chemistry is the study of compounds containing carbon. These compounds are fundamental to life and are found in a wide range of materials, from natural products like proteins and DNA to synthetic materials like plastics and pharmaceuticals.

1.2 Importance of Organic Chemistry

Organic chemistry is crucial in various fields, including pharmaceuticals, agriculture, materials science, and environmental science. Understanding organic compounds helps us develop new drugs, create sustainable materials, and protect the environment.

Chapter 2: Structure and Bonding in Organic Molecules

2.1 Carbon: The Central Atom

Carbon has four valence electrons, allowing it to form four covalent bonds. This versatility enables the formation of a vast array of organic compounds.

2.2 Types of Bonds

- **Single Bonds**: Formed by the sharing of one pair of electrons.
- **Double Bonds**: Formed by the sharing of two pairs of electrons.
- **Triple Bonds**: Formed by the sharing of three pairs of electrons.

Example: Methane (CH_4)

Methane is the simplest organic compound, consisting of one carbon atom bonded to four hydrogen atoms through single bonds.

Carbon: The Central Atom

2.1 Carbon: The Central Atom

Carbon is a unique and versatile element that forms the backbone of organic chemistry. Its ability to form a wide variety of compounds is due to its electronic configuration and bonding properties.

2.1.1 Electronic Configuration

Carbon has an atomic number of 6, which means it has 6 electrons. Its electron configuration is $1s^2\ 2s^2\ 2p^2$. The outermost shell (valence shell) contains 4 electrons, which are available for bonding.

2.1.2 Valence Electrons and Bonding

Carbon's four valence electrons allow it to form four covalent bonds. This ability to form multiple bonds with other atoms, including other carbon atoms, enables the creation of complex and diverse molecular structures.

2.1.3 Types of Bonds Formed by Carbon

Carbon can form different types of covalent bonds, including:

- **Single Bonds**: Formed by the sharing of one pair of electrons.
- **Double Bonds**: Formed by the sharing of two pairs of electrons.
- **Triple Bonds**: Formed by the sharing of three pairs of electrons.

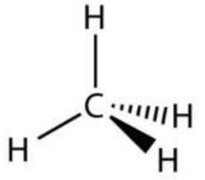
2.1.4 Hybridization

To understand the bonding in carbon compounds, it is essential to consider hybridization. Carbon can undergo sp^3, sp^2, and sp hybridization, which affects the geometry and reactivity of the molecule.

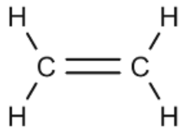
- **sp^3 Hybridization**: Forms tetrahedral geometry, as seen in alkanes.
- **sp^2 Hybridization**: Forms trigonal planar geometry, as seen in alkenes.
- **sp Hybridization**: Forms linear geometry, as seen in alkynes.

2.1.5 Examples of Carbon Compounds

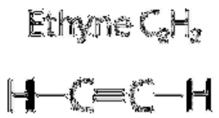
1. **Methane (CH_4)**
   - **Structure**: One carbon atom bonded to four hydrogen atoms through single bonds.
   - **Hybridization**: sp^3
   - **Geometry**: Tetrahedral
   - **Example**: Methane is the simplest alkane and a major component of natural gas.



2. **Ethene (C_2H_4)**
   - **Structure**: Two carbon atoms bonded to each other with a double bond and each carbon bonded to two hydrogen atoms.
   - **Hybridization**: sp^2
   - **Geometry**: Trigonal planar
   - **Example**: Ethene is an important industrial chemical used in the production of plastics.



3. **Ethyne (C_2H_2)**
   - **Structure**: Two carbon atoms bonded to each other with a triple bond and each carbon bonded to one hydrogen atom.
   - **Hybridization**: sp
   - **Geometry**: Linear
   - **Example**: Ethyne is used in welding and cutting metals due to its high energy content.



2.1.6 Versatility of Carbon

The ability of carbon to form long chains, rings, and complex structures with other elements (such as hydrogen, oxygen, nitrogen, and sulfur) makes it the central atom in organic chemistry. This versatility is crucial for the formation of biomolecules like carbohydrates, proteins, lipids, and nucleic acids, which are essential for life.

2.1.7 Conclusion

Carbon's unique bonding properties and ability to form a wide variety of compounds make it the central atom in organic chemistry. Understanding carbon's role in molecular structures and reactions is fundamental to studying organic chemistry and its applications in various fields.

Exercise 1

1. Provide the Lewis notation for the following compounds: CO_2, NH_4^+, F_2O, BH_3.
   Given: Z(H) = 1, Z(B) = 5, Z(C) = 6, Z(N) = 7, Z(O) = 8, Z(F) = 9.
2. Based on the electronic structures of sulfur and phosphorus atoms, explain the formation of the molecules SF_6 and PCl_5.
   Given: Z(Cl) = 17, Z(S) = 16, and Z(P) = 15.
3. Which of these compounds do not follow the octet rule?

Exercise 2

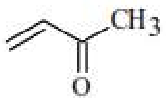
Consider the following organic molecule: CH_3-CO-CH=CH-CN

1. Provide the expanded form of this molecule.
2. Specify the hybridization states of the C, O, and N atoms.
3. Specify the atoms that are in the same plane.

Exercise 3

From the following structures:

1. Determine the hybridization state of each atom.
2. Determine the geometry of each molecule.

1°


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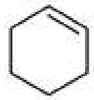

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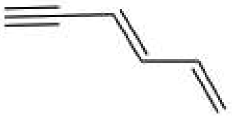
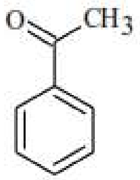


4°


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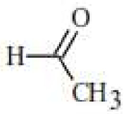


6° H_3C-NH_2

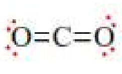
7° CO_2

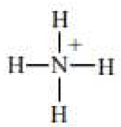
8° HCN

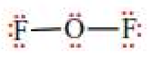
Solutions

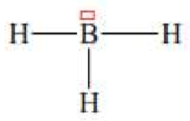
Exercise 1

1. **Lewis Notation of Compounds: CO_2, NH_4^+, F_2O, BH_3**
   - **CO_2**: For C, Z = 6, $1s^2\ 2s^2\ 2p^2$. There are 4 valence electrons. For O, Z = 8, $1s^2\ 2s^2\ 2p^4$. There are 6 valence electrons. Total: $4 + (2 \times 6) = 16$ valence electrons, hence 8 pairs.
   - **NH_4^+**: For H, Z = 1, $1s^1$. There is 1 valence electron. For N, Z = 7, $1s^2\ 2s^2\ 2p^3$. There are 5 valence electrons. Total: $(4 \times 1) + 5 - 1 = 8$ valence electrons, hence 4 pairs.
   - **F_2O**: For F, Z = 9, $1s^2\ 2s^2\ 2p^5$. There are 7 valence electrons. For O, Z = 8, $1s^2\ 2s^2\ 2p^4$. There are 6 valence electrons. Total: $6 + (2 \times 7) = 20$ valence electrons, hence 10 pairs.
   - **BH_3**: For B, Z = 5, $1s^2\ 2s^2\ 2p^1$. There are 3 valence electrons. Each H contributes one valence electron. Total: $3 + 3 = 6$ valence electrons, hence 3 pairs.





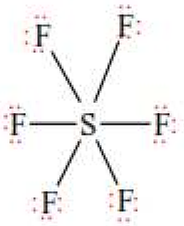


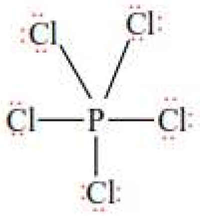


2. **Formation of Molecules SF_6 and PCl_5**
   - **SF_6**
     - Ground state: S (Z = 16): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4\ 3d^0$
     - Excited state: S*(Z = 16): $1s^2\ 2s^2\ 2p^6\ 3s^1\ 3p^3\ 3d^2$
       6 unpaired electrons
       $3s^2\ 3p^4\ 3d^0\ 3s^1\ 3p^3\ 3d^2$
       Ground state Excited state

- **PCl_5**
  - Ground state: P (Z = 15): $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3\ 3d^0$
  - Excited state: P*(Z = 15): $1s^2\ 2s^2\ 2p^6\ 3s^1\ 3p^3\ 3d^1$
    5 unpaired electrons
    $3s^2\ 3p^3\ 3d^0\ 3s^1\ 3p^3\ 3d^1$
    Ground state Excited state

Sulfur and phosphorus are atoms from the third period. They can accommodate more than 8 electrons by using 3d atomic orbitals.

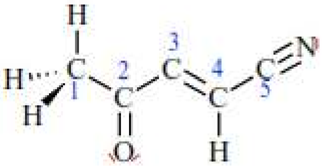




3. The octet rule is not satisfied for the compounds BH_3, SF_6, and PCl_5.

Exercise 2

1. Expanded form of the molecule CH_3-CO-CH=CH-CN



2. Hybridization states of atoms: C, O, and N

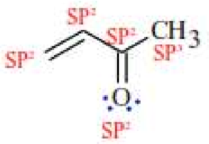
Atom	C1	C2	C3	C4	C5	O	N
Hybridization	Sp^3	Sp^2	Sp^2	Sp^2	Sp	Sp^2	Sp

3. All atoms are in the same plane except the two hydrogens of the CH_3 group.

Exercise 3

1 and 2

1°

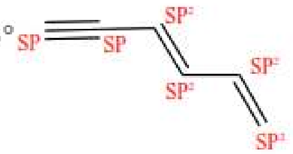


Molecular spatial

2°

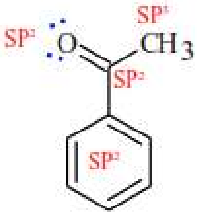
Molecular spatial

3°



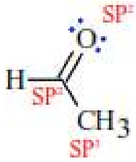
Planar molecule

4°



Molecular spatial

5°



Molecular spatial

6°

Molecular spatial

7°

8°

Linear molecule

Linear molecule

Supplementary Exercise

Exercise 1: Electron Configuration

Question: Write the ground-state electron configuration for the following elements:

- Oxygen (O)
- Nitrogen (N)
- Sulfur (S)

Solution:

- **Oxygen (O):** Oxygen has an atomic number of 8, meaning it has 8 electrons. The electron configuration is $1s^2\ 2s^2\ 2p^4$

- **Nitrogen (N):** Nitrogen has an atomic number of 7, meaning it has 7 electrons. The electron configuration is $1s^2\ 2s^2\ 2p^3$
- .
- **Sulfur (S):** Sulfur has an atomic number of 16, meaning it has 16 electrons. The electron configuration is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$

Exercise 2: Valence Electrons and Bonding

Question: Determine the number of valence electrons for the following elements and predict the number of covalent bonds they can form:

- Magnesium (Mg)
- Cobalt (Co)
- Selenium (Se)

Solution:

- **Magnesium (Mg):** Magnesium is in group 2A of the periodic table, so it has 2 valence electrons. It typically forms 2 covalent bonds

- **Cobalt (Co):** Cobalt is a transition metal. It has 2 electrons in the 4s subshell and 7 electrons in the 3d subshell. Transition metals can form a variable number of bonds, but typically they can form up to 6 covalent bonds
- **Selenium (Se):** Selenium is in group 6A of the periodic table, so it has 6 valence electrons. It typically forms 2 covalent bonds

Exercise 3: Drawing Electron-Dot and Line-Bond Structures

Question: Draw the electron-dot structure and line-bond structure for the following molecules:

- Chloroform ($CHCl_3$)
- Hydrogen sulfide (H_2S)
- Methylamine (CH_3NH_2)

Solution:

- **Chloroform ($CHCl_3$):**
  - **Electron-dot structure:** Carbon has 4 valence electrons, hydrogen has 1, and each chlorine has 7. Two electrons are used for each single bond, and the remaining electrons are used to achieve a noble gas configuration for all atoms

- **Line-bond structure:** Replace the electron dots between two atoms with a line
- **Hydrogen sulfide (H_2S):**

  - **Electron-dot structure:** Sulfur has 6 valence electrons, and each hydrogen has 1. Two electrons are used for each single bond, and the remaining electrons form lone pairs on sulfur

- **Line-bond structure:** Replace the electron dots between two atoms with a line
- **Methylamine (CH_3NH_2):**

- **Electron-dot structure:** Carbon has 4 valence electrons, nitrogen has 5, and each hydrogen has 1. Two electrons are used for each single bond, and the remaining electrons form lone pairs on nitrogen

- **Line-bond structure:** Replace the electron dots between two atoms with a line

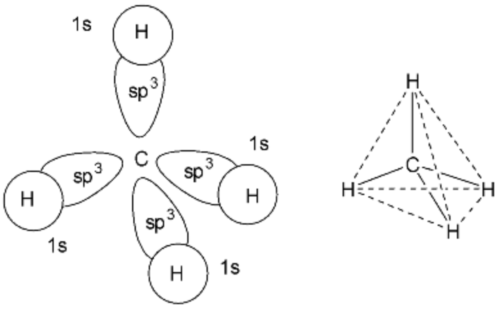
Exercise 4: Hybridization and Molecular Geometry

Question: Determine the hybridization and molecular geometry of the central atom in the following molecules:

- Methane (CH_4)
- Ethene (C_2H_4)
- Ethyne (C_2H_2)

Solution:

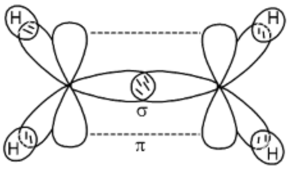
- **Methane (CH_4):**
  - **Hybridization:** sp^3
  - **Molecular geometry:** Tetrahedral

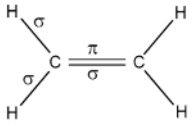


Formation and structure of methane

- **Ethene (C_2H_4):**

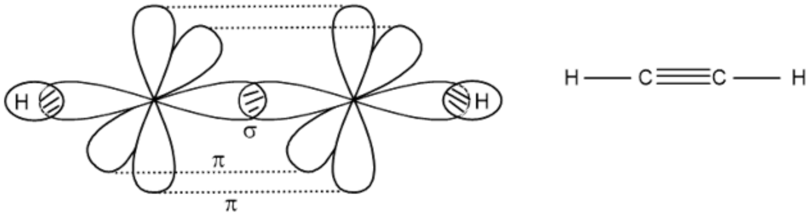
- **Hybridization:** sp^2
- **Molecular geometry:** Trigonal planar





Trigonal Planar shape

- **Ethyne (C_2H_2):**
  - **Hybridization:** sp
  - **Molecular geometry:** Linear



Chapter 3: Functional Groups

3.1 Definition

Functional groups are specific groups of atoms within organic molecules that are responsible for the characteristic chemical reactions of those molecules.

3.2 Common Functional Groups

- **Alcohols** (-OH)
- **Aldehydes** (-CHO)
- **Ketones** (>C=O)
- **Carboxylic Acids** (-COOH)
- **Amines** ($-NH_2$)
- **Ethers** (-O-)

Example: Ethanol (C_2H_5OH)

Ethanol contains an alcohol functional group (-OH) attached to an ethyl group (C_2H_5).

Functional Groups in Organic Chemistry

Functional groups are specific groups of atoms within organic molecules that are responsible for the characteristic chemical reactions of those molecules. Here is a detailed overview of some common functional groups:

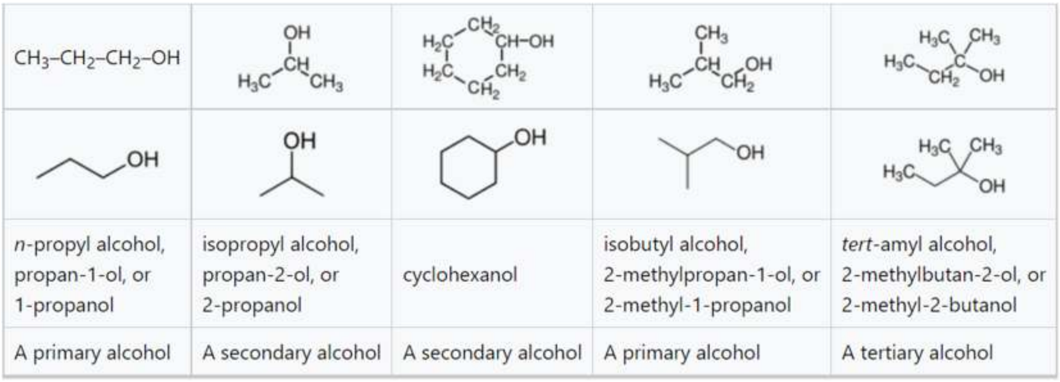
1. Alcohols (-OH)

Structure: An -OH group attached to a carbon atom.
General Formula: R-OH
Properties:

- Alcohols are polar due to the presence of the -OH group.
- They can form hydrogen bonds, which affects their boiling points and solubility in water.

Example: Ethanol (C_2H_5OH)

- **Structure**: CH_3CH_2OH
- **Use**: Ethanol is used as a solvent, in alcoholic beverages, and as a fuel.



$CH_3-CH_2-CH_2-OH$				
n-propyl alcohol, propan-1-ol, or 1-propanol	isopropyl alcohol, propan-2-ol, or 2-propanol	cyclohexanol	isobutyl alcohol, 2-methylpropan-1-ol, or 2-methyl-1-propanol	*tert*-amyl alcohol, 2-methylbutan-2-ol, or 2-methyl-2-butanol
A primary alcohol	A secondary alcohol	A secondary alcohol	A primary alcohol	A tertiary alcohol

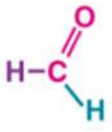
2. Aldehydes (-CHO)

Structure: A carbonyl group (-C=O) attached to a carbon atom and a hydrogen atom.
General Formula: R-CHO
Properties:

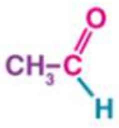
- Aldehydes are polar and can participate in hydrogen bonding.
- They are reactive due to the presence of the carbonyl group.

Example: Acetaldehyde (CH_3CHO)

- **Structure**: CH_3CHO
- **Use**: Acetaldehyde is used in the production of acetic acid and perfumes.
-



Methanal



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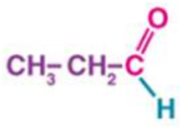
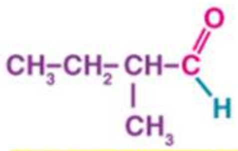


Propanal



2-Methylbutanal

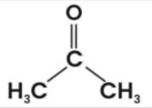
3. Ketones (>C=O)

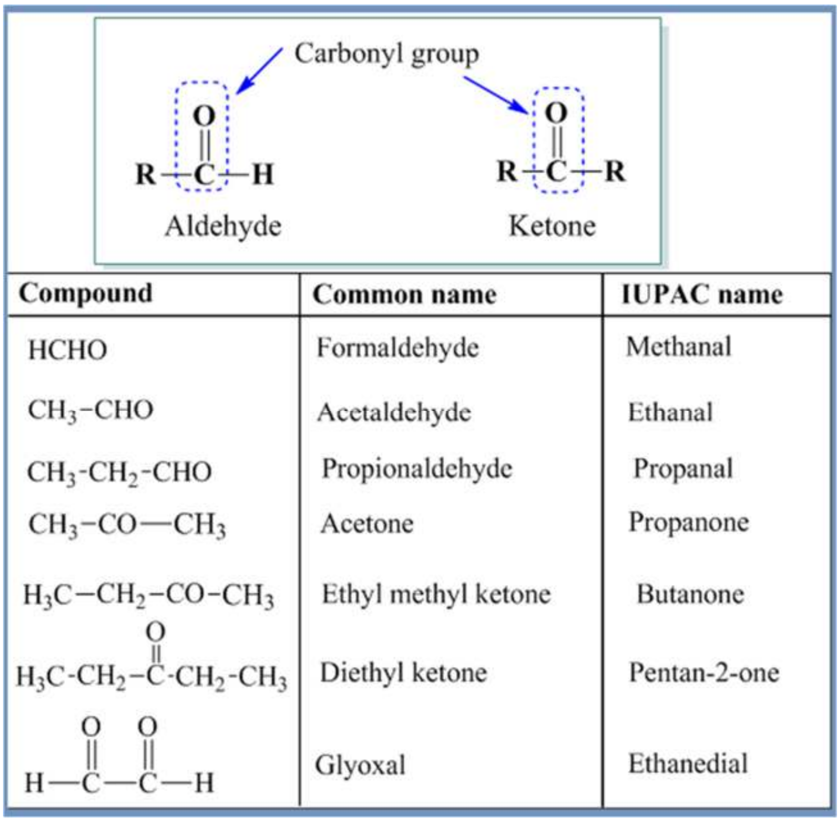
Structure: A carbonyl group (-C=O) attached to two carbon atoms.
General Formula: R-CO-R'
Properties:

- Ketones are polar and can participate in hydrogen bonding.
- They are less reactive than aldehydes due to steric hindrance.

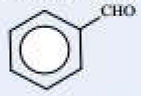
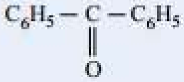
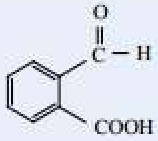
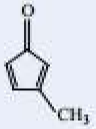
Example: Acetone (CH_3COCH_3)

- **Structure**: CH_3COCH_3
- **Use**: Acetone is a common solvent used in nail polish remover and as a cleaning agent.

Molecular Formula	IUPAC Name	Common Name	Structure
CH_3COCH_3	Propan-2-one	Acetone	



Compound	Common name	IUPAC name
HCHO	Formaldehyde	Methanal
CH_3-CHO	Acetaldehyde	Ethanal
CH_3-CH_2-CHO	Propionaldehyde	Propanal
$CH_3-CO-CH_3$	Acetone	Propanone
$H_3C-CH_2-CO-CH_3$	Ethyl methyl ketone	Butanone
$H_3C-CH_2-\overset{O}{\overset{\|}{C}}-CH_2-CH_3$	Diethyl ketone	Pentan-2-one
$H-\overset{O}{\overset{\|}{C}}-\overset{O}{\overset{\|}{C}}-H$	Glyoxal	Ethanedial

Benzaldehyde  phenyl methanal	phenyl	meth	an$\cancel{e}$	al
Acetone / Dimethyl ketone $CH_3 - CO - CH_3$ propanone	-	prop	an$\cancel{e}$	one
Mesityl oxide $(CH_3)_2C = CHCOCH_3$ 4 – methylpent-3-en-2-one	4 – methyl	pent	3-en$\cancel{e}$	2-one
Methyl Phenyl ketone  $C_6H_5 - \underset{\underset{O}{\parallel}}{C} - CH_3$ Acetophenone (PIN)* 1-phenylethan-1-one	1-phenyl	eth	an$\cancel{e}$	1-one
Diphenyl ketone  $C_6H_5 - \underset{\underset{O}{\parallel}}{C} - C_6H_5$ Benzophenone (PIN)* Diphenylmethanone	Diphenyl	meth	an$\cancel{e}$	one
 $CH_3 - CH_2 - \overset{\overset{O}{\parallel}}{C} - CH_2 - CHO$ 3 - oxopentanal	3 - oxo	pent	an$\cancel{e}$	al
 2 – formylbenzoicacid	2 – formyl	benz	-	oicacid
 3 -methylcyclopent-2,4-dien-1-one	3 -methyl	cyclopent	2, 4 dien$\cancel{e}$	1-one

4. Carboxylic Acids (-COOH)

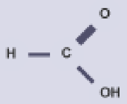
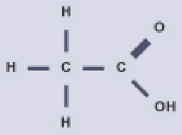
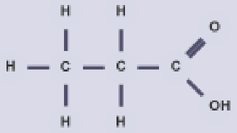
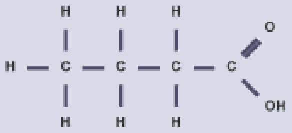
Structure: A carbonyl group (-C=O) attached to a hydroxyl group (-OH).
General Formula: R-COOH
Properties:

- Carboxylic acids are acidic due to the presence of the -COOH group.

- They can donate a proton (H^+) to form a carboxylate ion.

Example: Acetic Acid (CH_3COOH)

- **Structure**: CH_3COOH
- **Use**: Acetic acid is the main component of vinegar and is used in the production of polymers and pharmaceuticals.

Name	Molecular Formula	Structural Formula	State at room temperature & pressure
Methanoic Acid	HCOOH		Liquid
Ethanoic Acid	CH_3COOH		Liquid
Propanoic Acid	C_2H_5COOH		Liquid
Butanoic Acid	C_3H_7COOH		Liquid

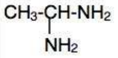
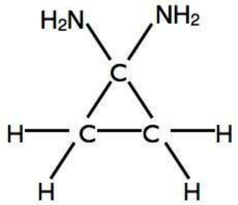
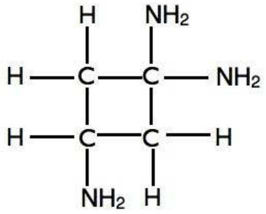
5. Amines ($-NH_2$)

Structure: A nitrogen atom bonded to one or more hydrogen atoms and carbon atoms.
General Formula: $R-NH_2$ (primary amine), R-NHR' (secondary amine), R-NR'R" (tertiary amine)
Properties:

- Amines are basic due to the presence of the lone pair of electrons on the nitrogen atom.
- They can form hydrogen bonds, which affects their boiling points and solubility in water.

Example: Methylamine (CH_3NH_2)

- **Structure**: CH_3NH_2
- **Use**: Methylamine is used in the production of pharmaceuticals and as a precursor to other chemicals.

Structural formula	IUPAC name
$NH_2\text{-}CH_2\text{-}CH_2\text{-}NH_2$	Ethane-1,2-diamine
 $CH_3\text{-}\underset{NH_2}{CH}\text{-}NH_2$	Ethane-1,1-diamine
$NH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}NH_2$	Propane-1,3-diamine
	Cyclopropane-1,1-diamine
	Cyclobutane-1,1,3-triamine

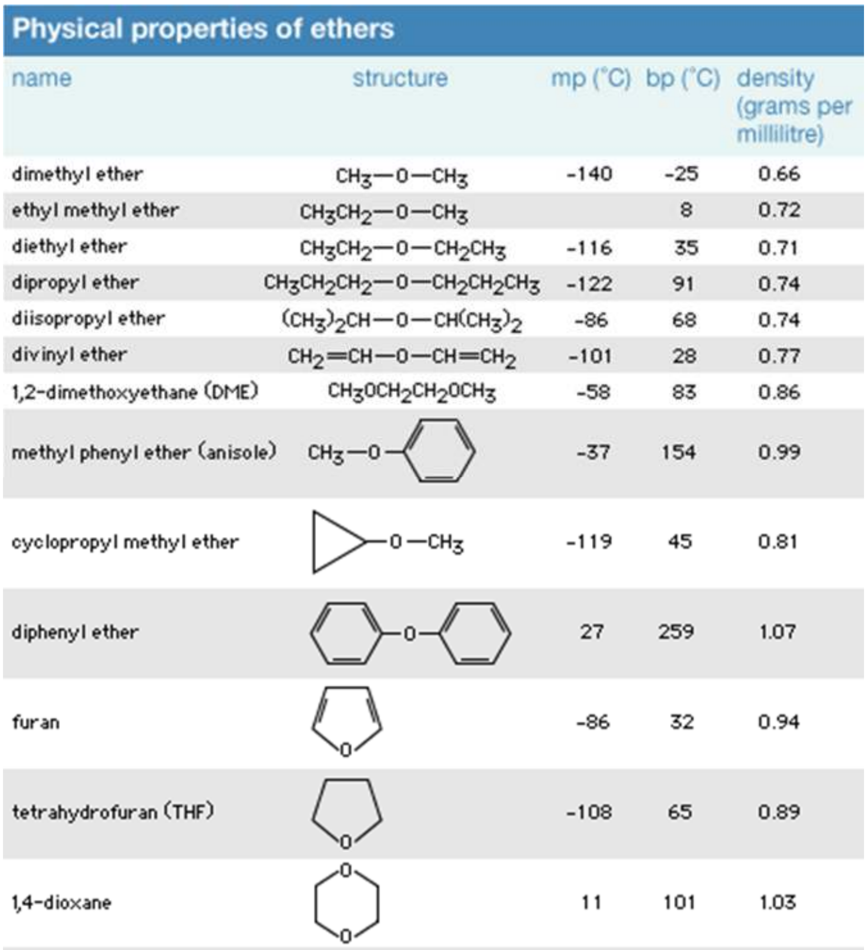
6. Ethers (-O-)

Structure: An oxygen atom bonded to two carbon atoms.
General Formula: R-O-R'
Properties:

- Ethers are relatively non-polar and do not form hydrogen bonds.
- They are generally less reactive than alcohols and carboxylic acids.

Example: Diethyl Ether ($CH_3CH_2OCH_2CH_3$)

- **Structure**: $CH_3CH_2OCH_2CH_3$
- **Use**: Diethyl ether is used as a solvent and historically as an anesthetic.



Physical properties of ethers

name	structure	mp (°C)	bp (°C)	density (grams per millilitre)
dimethyl ether	CH_3-O-CH_3	-140	-25	0.66
ethyl methyl ether	$CH_3CH_2-O-CH_3$		8	0.72
diethyl ether	$CH_3CH_2-O-CH_2CH_3$	-116	35	0.71
dipropyl ether	$CH_3CH_2CH_2-O-CH_2CH_2CH_3$	-122	91	0.74
diisopropyl ether	$(CH_3)_2CH-O-CH(CH_3)_2$	-86	68	0.74
divinyl ether	$CH_2=CH-O-CH=CH_2$	-101	28	0.77
1,2-dimethoxyethane (DME)	$CH_3OCH_2CH_2OCH_3$	-58	83	0.86
methyl phenyl ether (anisole)	CH_3-O-	-37	154	0.99
cyclopropyl methyl ether	$-O-CH_3$	-119	45	0.81
diphenyl ether	$-O-$	27	259	1.07
furan	O	-86	32	0.94
tetrahydrofuran (THF)	O	-108	65	0.89
1,4-dioxane	O O	11	101	1.03

Summary of Functional Groups

Functional Group	Structure	General Formula	Example	Example Structure	Use
Alcohols	-OH	R-OH	Ethanol	CH_3CH_2OH	Solvent, fuel, beverages
Aldehydes	-CHO	R-CHO	Acetaldehyde	CH_3CHO	Production of acetic acid, perfumes
Ketones	>C=O	R-CO-R'	Acetone	CH_3COCH_3	Solvent, cleaning agent
Carboxylic Acids	-COOH	R-COOH	Acetic Acid	CH_3COOH	Vinegar, polymers, pharmaceuticals
Amines	$-NH_2$	$R-NH_2$	Methylamine	CH_3NH_2	Pharmaceuticals, chemical precursor
Ethers	-O-	R-O-R'	Diethyl Ether	$CH_3CH_2OCH_2CH_3$	Solvent, anesthetic

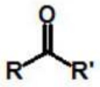
Major Organic Chemistry Functional Groups

Alkane

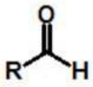
Alkene

Conjugated
Alkene

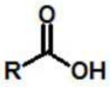
Alkyne



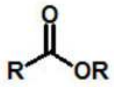
Ketone



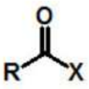
Aldehyde



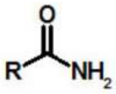
Carboxylic
Acid



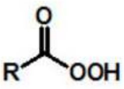
Ester



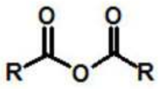
Acid Halide



Amide



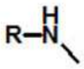
Peroxy Acid



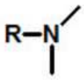
Anhydride

$R-NH_2$

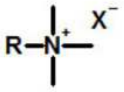
Primary
Amine



Secondary
Amine

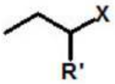


Tertiary
Amine

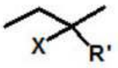


Quaternary
Ammonium Salt

Primary
Alkyl Halide



Secondary
Alkyl Halide



Tertiary
Alkyl Halide

R—OH

Alcohol

R—O—R

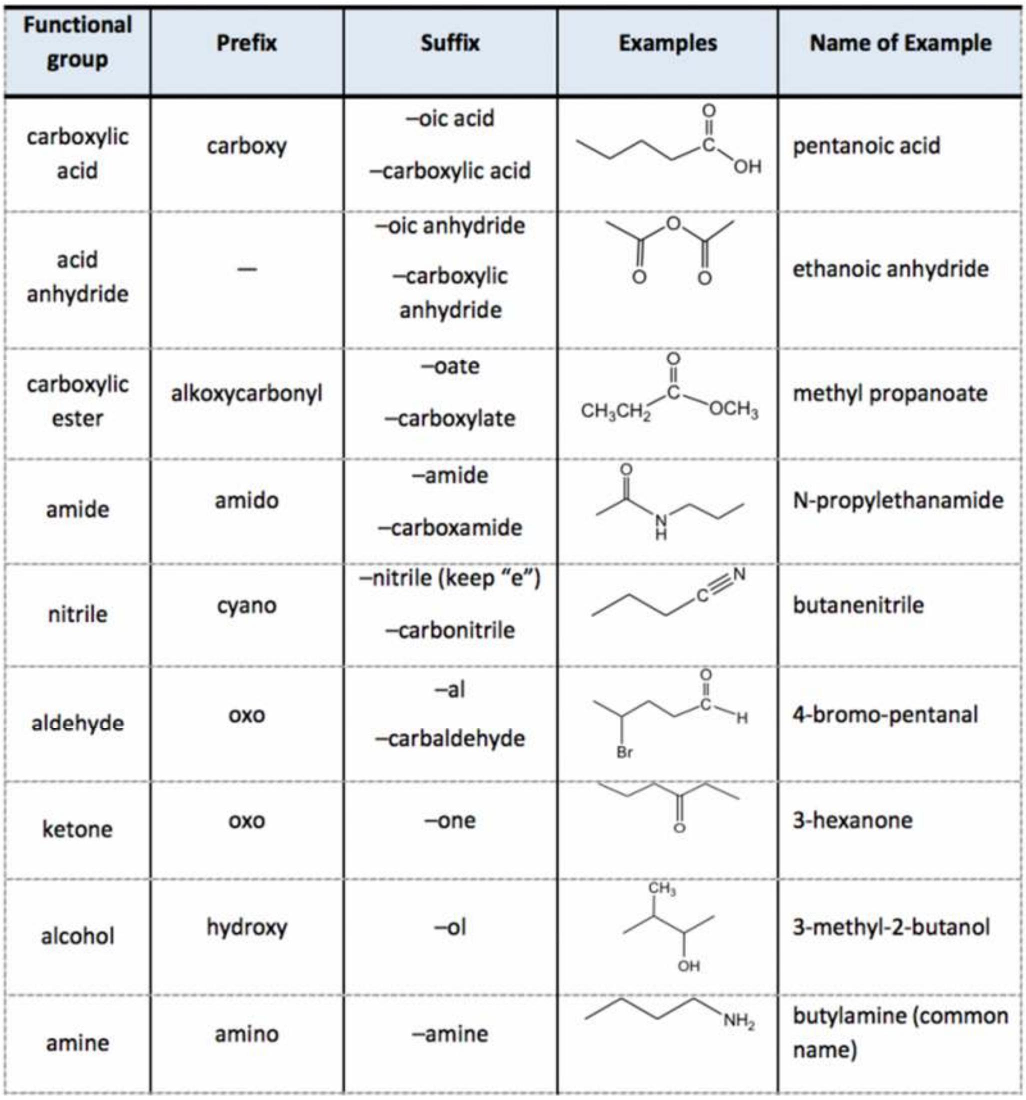
Ether

R—SH

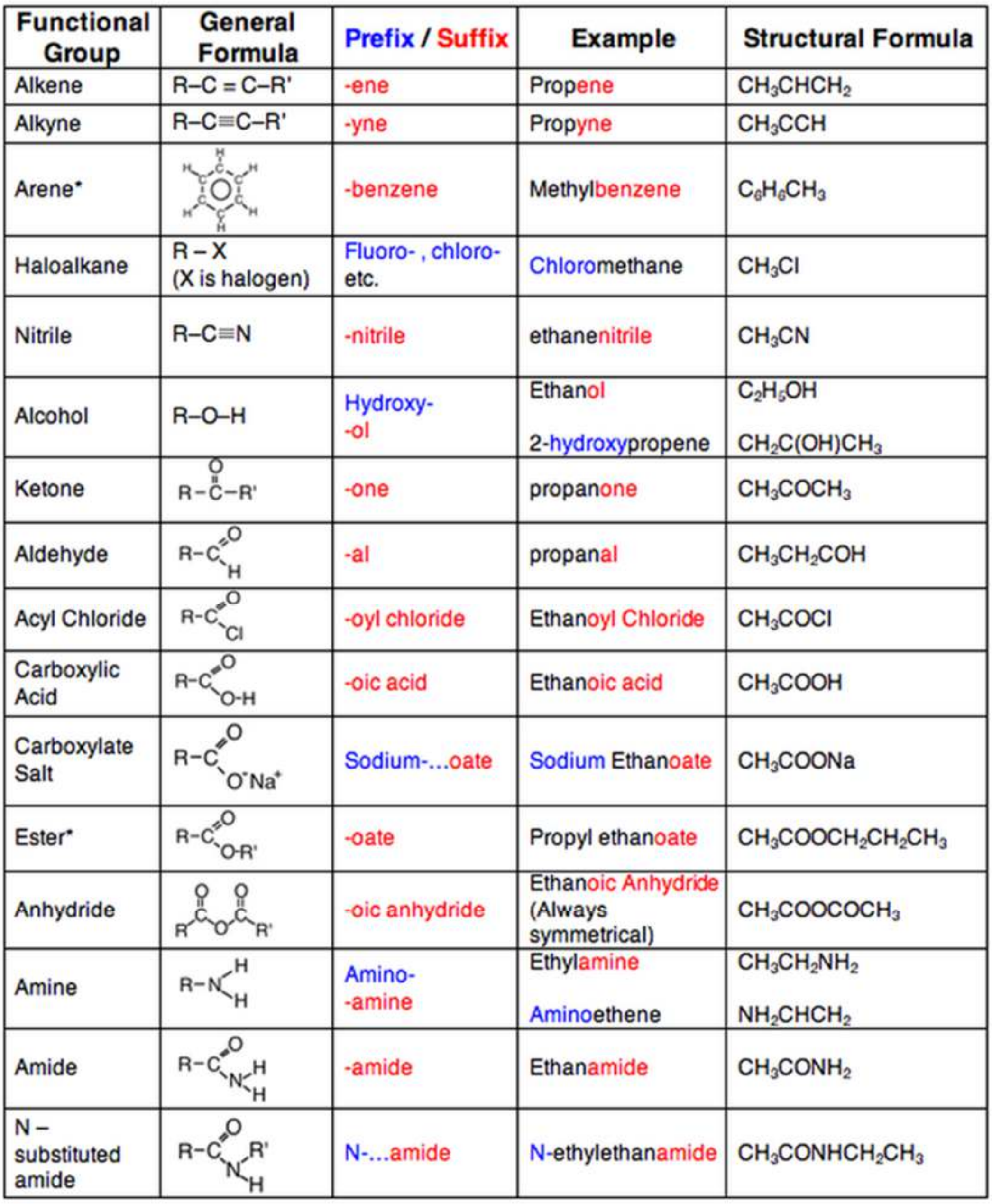
Thiol

R—S—R

Thioether



Functional group	Prefix	Suffix	Examples	Name of Example
carboxylic acid	carboxy	–oic acid –carboxylic acid		pentanoic acid
acid anhydride	—	–oic anhydride –carboxylic anhydride		ethanoic anhydride
carboxylic ester	alkoxycarbonyl	–oate –carboxylate		methyl propanoate
amide	amido	–amide –carboxamide		N-propylethanamide
nitrile	cyano	–nitrile (keep “e”) –carbonitrile		butanenitrile
aldehyde	oxo	–al –carbaldehyde		4-bromo-pentanal
ketone	oxo	–one		3-hexanone
alcohol	hydroxy	–ol		3-methyl-2-butanol
amine	amino	–amine		butylamine (common name)

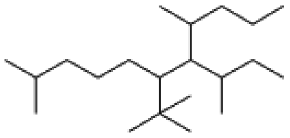


Functional Group	General Formula	Prefix / Suffix	Example	Structural Formula
Alkene	$R-C=C-R'$	-ene	Propene	CH_3CHCH_2
Alkyne	$R-C\equiv C-R'$	-yne	Propyne	CH_3CCH
Arene*		-benzene	Methylbenzene	$C_6H_6CH_3$
Haloalkane	R – X (X is halogen)	Fluoro- , chloro- etc.	Chloromethane	CH_3Cl
Nitrile	$R-C\equiv N$	-nitrile	ethanenitrile	CH_3CN
Alcohol	$R-O-H$	Hydroxy- -ol	Ethanol 2-hydroxypropene	C_2H_5OH $CH_2C(OH)CH_3$
Ketone	$R-\overset{O}{\overset{\|}{C}}-R'$	-one	propanone	CH_3COCH_3
Aldehyde	$R-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow H}$	-al	propanal	CH_3CH_2COH
Acyl Chloride	$R-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow Cl}$	-oyl chloride	Ethanoyl Chloride	CH_3COCl
Carboxylic Acid	$R-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow O-H}$	-oic acid	Ethanoic acid	CH_3COOH
Carboxylate Salt	$R-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow O^-Na^+}$	Sodium-…oate	Sodium Ethanoate	CH_3COONa
Ester*	$R-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow O-R'}$	-oate	Propyl ethanoate	$CH_3COOCH_2CH_2CH_3$
Anhydride	$R-\overset{O}{\overset{\|}{C}}-O-\overset{O}{\overset{\|}{C}}-R'$	-oic anhydride	Ethanoic Anhydride (Always symmetrical)	$CH_3COOCOCH_3$
Amine	$R-N\genfrac{}{}{0pt}{}{\nearrow H}{\searrow H}$	Amino- -amine	Ethylamine Aminoethene	$CH_3CH_2NH_2$ NH_2CHCH_2
Amide	$R-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow NH_2}$	-amide	Ethanamide	CH_3CONH_2
N – substituted amide	$R-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow N(H)R'}$	N-…amide	N-ethylethanamide	$CH_3CONHCH_2CH_3$

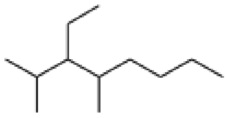
Exercise 1

Name the following compounds:

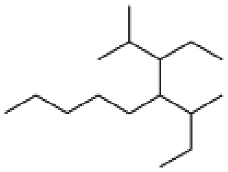
1°



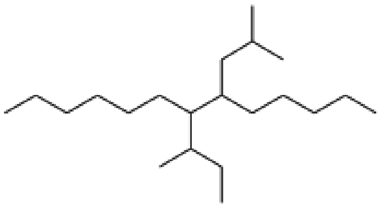
2°



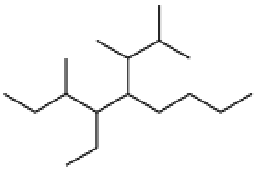
3°



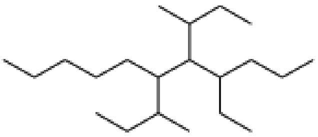
4°



5°

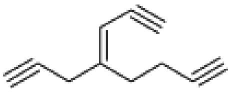


6°

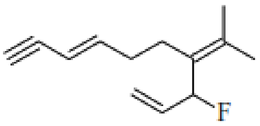


7°

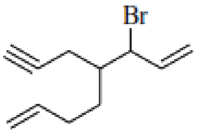
8°



9°



10°



Exercise 2

Name the following compounds:

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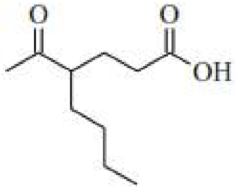
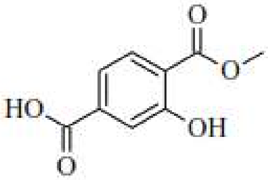


2:



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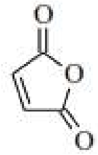

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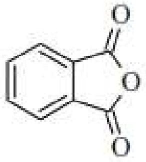
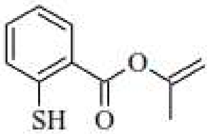
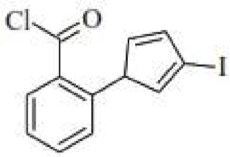


5:

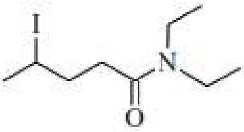
6:



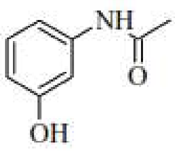
7:



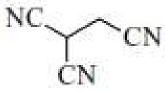
8:



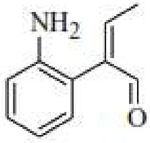
9:



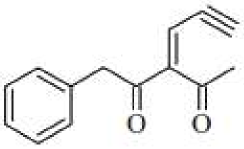
10:



11:

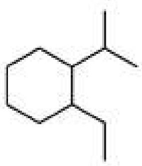


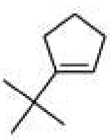
12:

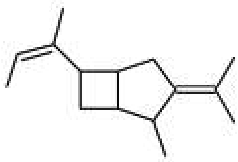


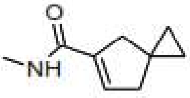
Exercise 3

Name the following compounds:





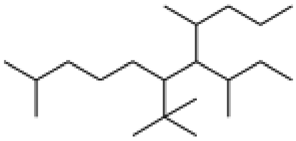




Solutions

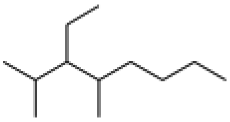
Exercise 1

1°



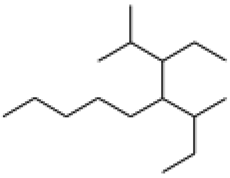
6-tert-butyl-2,8-dimethyl-7-(1-methylpropyl)undecane

2°



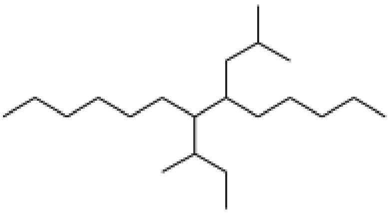
3-ethyl-2,4-dimethyloctane

3°



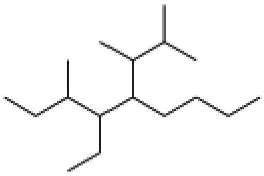
3-ethyl-2-methyl-4(2-methylpropyl)nonane

4°



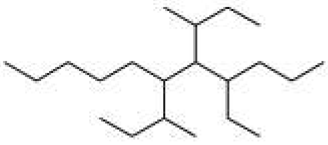
7-(1-methylpropyl)-6-(2-methylpropyl)tridecane

5°



5-(1,2-dimethylpropyl)-4-ethyl-3-methylnonane

6°

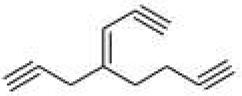


4-ethyl-5,6-bis(1-methylpropyl)undecane

7°

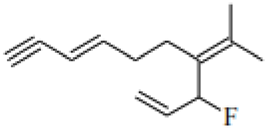
hept-1-ene-6-yne

8°



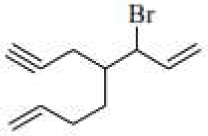
4-prop-2-ynyloct-3-ene-1,7-diyne

9°



8-fluoro-7-isopropylidenedeca-3,9-diene-1-yne

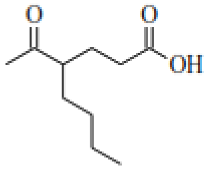
10°



3-bromo-4-prop-2-énylocta-1,7-diene

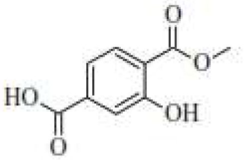
Exercise 2 1:

1:



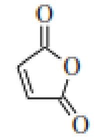
4-acetyloctanoic acid

2:



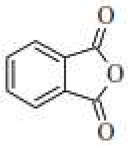
3-hydroxy-4-(methoxycarbonyl)benzoic acid

3:



But-2-ene-1,4-dioic anhydride

4:

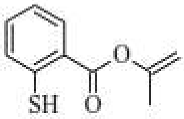


Benzene-1,2-dicarboxylic anhydride

5:

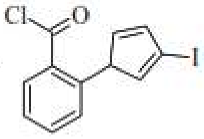
3-methylbutyl acetate

6:



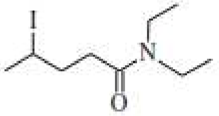
2-mercaptobenzoyl isopropyl ester

7:



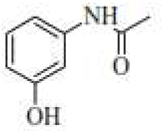
Chloride of 2-(3-iodocyclopenta-2,4-dienyl)benzoyl

8:



N,N-diethyl-4-iodopentanamide

9:

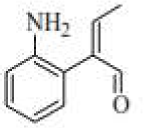


N-(3-hydroxyphenyl)acetamide

10:

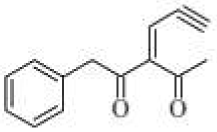
Ethane-1,1,2-tricarbonitrile

11:



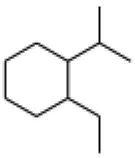
2-(2-aminophenyl)but-2-enal

12:

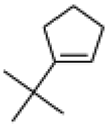


1-phenyl-3-(prop-2-ynylidene)pentane-2,4-dione

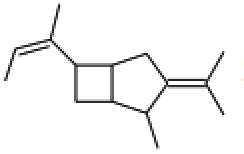
Exercise 3



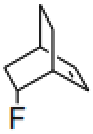
1-ethyl-2-isopropylcyclohexane



1-tert-butylcyclopentene

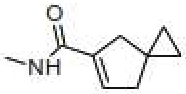


3-isopropylidene-2-methyl-6-(1-methylpropenyl)bicyclo[3.2.0]heptane



5-fluorobicyclo[2.2.2]oct-2-ene

6-cyano-1-(prop-2-enyl)spiro[2.4]heptane-5-carboxylic acid



N-methylspiro[2.4]hept-5-ene-5-carboxamide

Supplementary Exercise

EXERCICES Exercise 1: Name the following compounds according to the IUPAC nomenclature rules:

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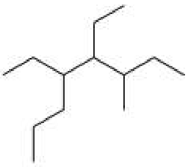
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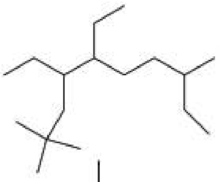
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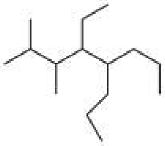
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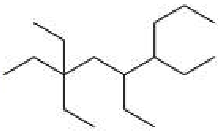
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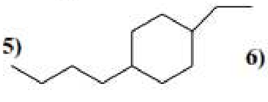
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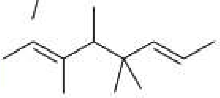
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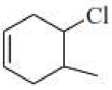

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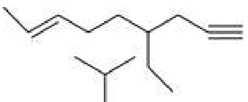
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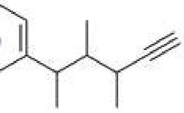
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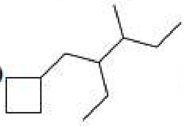
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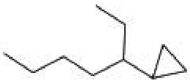
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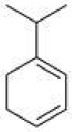
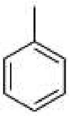


Exercise 2: Name the following aromatic compounds according to IUPAC:

1)

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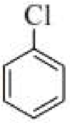

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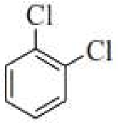

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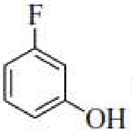

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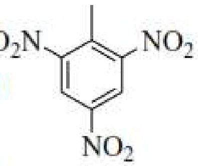

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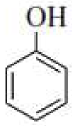

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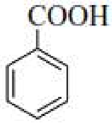

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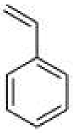
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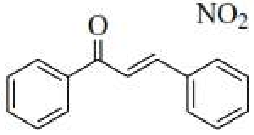


Exercise 3 : Name the following compounds according to IUPAC:

a) CH3-CH(OH)-CHCl-CH2 -CH(CH3)2
b) (C2H5)2N-CH2-CH=CH-CH3
c) OH-CH2-CH(Et)-CH2-CHO
d) CH3-CO-CH2-C≡C-CH(CH3)NH2
e) H2N-CO-CH2-CH(CN)-CH(iPr)-C(OH)2-CH3
f) HOOC-CH=CH2
g) CHO-CH=CH-COOH
h) (CH3)2CH-CH(CH2Cl)-CH2CN

Exercise 4: Draw the semi-developed formulas of the following molecules:

a) 4-propylhex-4-ene-3-one
b) 3-amino-4-ethylhex-5-enoic acid
c) 2,3,3-triethylheptane

d) 1-amino-4-(cyclobut-2-enyl)-4-methoxybutan-1-ol
e) Butadione
f) 4-(2-hydroxyethyl)hex-5-enoic acid
g) N,N-dimethylbutanamide
h) 5-amino-3-(2-hydroxyethyl)heptanoic acid
i) Para-methyl phenol
j) 3-amino-2-methoxybutanoate of isopropyl
k) 5-(N-methylamino)-3-vinylcyclohex-3-enone
l) 5-(N,N-dimethylamino)-3-ethoxy-3-chloro-2-phenylhexanoate of tert-butyl

Exercise 5: Provide the topological formulas of the following molecules:

a) 4-propylhex-4-ene-3-one
b) 2,3,3-triethylheptane
c) 3,5-diethyl-2-propyloctane
d) 3-amino-4-ethylhex-5-enoic acid

Chapter 4: Nomenclature of Organic Compounds

4.1 IUPAC Naming Rules

The International Union of Pure and Applied Chemistry (IUPAC) provides a systematic way to name organic compounds based on their structure.

Example: 2-Methylpropane

This compound is named based on the longest carbon chain (3 carbons, propane) with a methyl group attached to the second carbon.

4.1 IUPAC Naming Rules

The International Union of Pure and Applied Chemistry (IUPAC) has established a set of rules for the systematic naming of organic compounds. These rules ensure that each compound has a unique and unambiguous name. Here are the key steps and guidelines for IUPAC nomenclature:

1. Identify the Longest Carbon Chain

- **Longest Chain Rule**: The parent hydrocarbon chain is the longest continuous chain of carbon atoms in the molecule. This chain can be straight or branched
- **Example**: For a compound with a chain of 5 carbons, the root name would be "pentane".

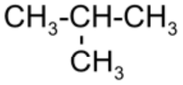
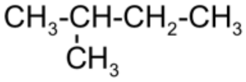
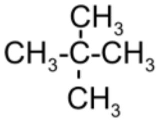
2. Number the Carbon Atoms

- **Lowest Set of Locants**: Number the carbon atoms in the parent chain starting from the end nearest to the substituent or functional group. This ensures the lowest possible numbers for the substituents
- **Example**: If a substituent is attached to the second carbon in a 5-carbon chain, the numbering starts from the end closest to this substituent.

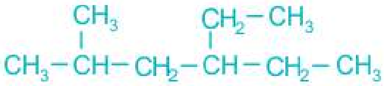
3. Identify and Name Substituents

- **Multiple Instances of the Same Substituent**: Use prefixes like "di-", "tri-", "tetra-", etc., to indicate the number of identical substituents

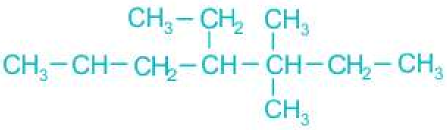
- **Different Substituents**: List substituents in alphabetical order, regardless of their position on the chain
- **Complex Substituents**: Name branched or complex substituents as substituted alkyl groups. The carbon attached to the parent chain is numbered as 1

Structure	IUPAC name	Common name
CH_4	Methane	Methane
CH_3CH_3	Ethane	Ethane
$CH_3CH_2CH_3$	Propane	Propane
$CH_3CH_2CH_2CH_3$	Butane	n-Butane
 $CH_3\text{-}\underset{CH_3}{CH}\text{-}CH_3$	2-Methyl propane	Isobutane
$CH_3CH_2CH_2CH_2CH_3$	Pentane	n-Pentane
 $CH_3\text{-}\underset{CH_3}{CH}\text{-}CH_2\text{-}CH_3$	2-Methyl butane	Isopentane
 $CH_3\text{-}\underset{CH_3}{\overset{CH_3}{C}}\text{-}CH_3$	2,2-Dimethyl propane	Neopentane

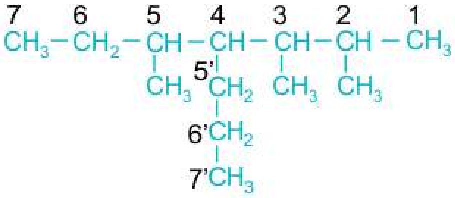
The examples of organic compounds area:


$CH_3-\overset{CH_3}{CH}-CH_2-\overset{CH_2-CH_3}{CH}-CH_2-CH_3$

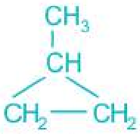
4-ethyl-2-methylhexane


$CH_3-CH-CH_2-\overset{CH_3-CH_2}{CH}-\underset{CH_3}{\overset{CH_3}{CH}}-CH_2-CH_3$

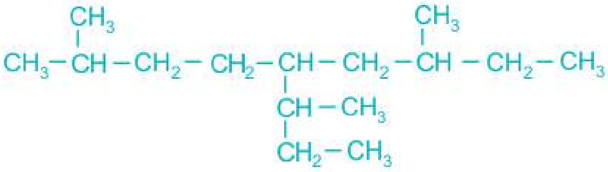
4-ethyl-3,3-dimethylheptane



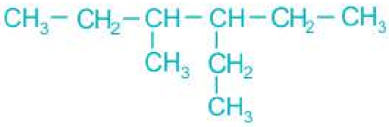
2,3,5-trimethyl-4-propylheptane
(NOT: 2,3-dimetyl-4-sec-butylheptane)



methylcyclopropane

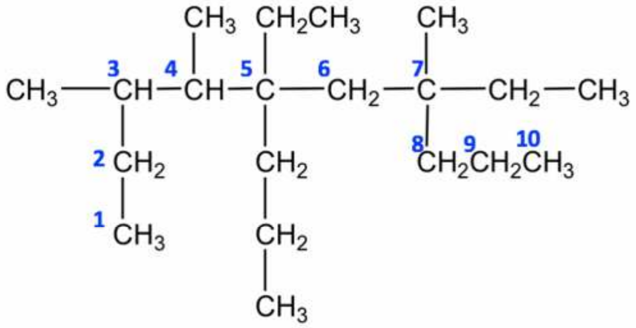


5-sec-butyl-2,7-dimethylnonane



3-ethyl-4-methylhexane

Nomenclature of Organic Compounds Examples



Find the parent chain correctly is the key step for naming this structure.

5,7-diethyl-3,4,7-trimethyl-5-propyldecane

4. Functional Groups

- **Primary Suffix**: Indicates the main functional group in the molecule. For example, "ane" for alkanes, "ene" for alkenes, and "yne" for alkynes

- **Secondary Suffix**: Used for additional functional groups. For example, "ol" for alcohols, "al" for aldehydes, and "one" for ketones

5. Naming Compounds with Multiple Functional Groups

- **Priority of Functional Groups**: Functional groups have a priority order. For example, carboxylic acids have higher priority than alcohols, which in turn have higher priority than alkenes

- **Example**: A compound with both a carboxylic acid and an alcohol group would be named as a carboxylic acid with an alcohol substituent.

6. Examples of IUPAC Names

- **Alkanes**: Methane (CH_4), Ethane (C_2H_6), Propane (C_3H_8), Butane (C_4H_{10})

- **Alkenes**: Ethene (C_2H_4), Propene (C_3H_6)
- **Alkynes**: Ethyne (C_2H_2)
- **Alcohols**: Propan-1-ol ($CH_3CH_2CH_2OH$), Propan-2-ol ($CH_3CHOHCH_3$)
- **Ethers**: Ethyl propyl ether ($CH_3CH_2OCH_2CH_2CH_3$)

7. Special Cases

- **Cyclic Compounds**: Use "cyclo-" as a prefix to indicate a ring structure. For example, cyclohexane for a 6-carbon ring

- **Halogenated Compounds**: Use prefixes like "fluoro-", "chloro-", "bromo-", and "iodo-" to indicate halogen substituents.

Chapter 5: Isomerism

5.1 Definition

Isomers are compounds with the same molecular formula but different structural arrangements.

5.2 Types of Isomerism

- **Structural Isomerism**: Different connectivity of atoms.
- **Stereoisomerism**: Same connectivity but different spatial arrangement.

Example: Butane and Isobutane

Butane ($CH_3CH_2CH_2CH_3$) and isobutane ($CH_3CH(CH_3)_2$) are structural isomers.

Chapter 5: Isomerism

5.1 Definition

Isomers are compounds with the same molecular formula but different structural arrangements. This means that while they have the same number and type of atoms, the way these atoms are connected or arranged in space differs, leading to distinct properties and behaviors.

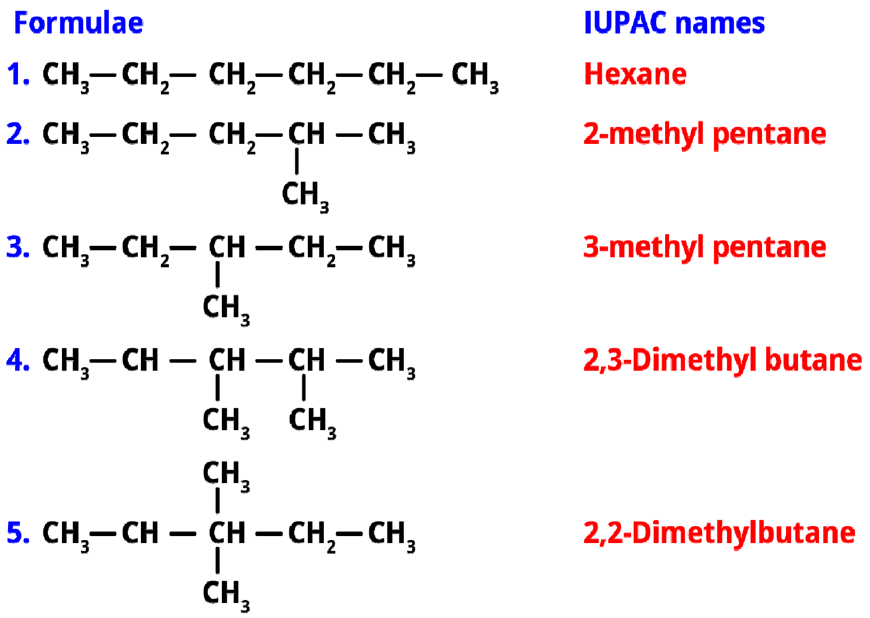
5.2 Types of Isomerism

5.2.1 Structural Isomerism

Structural isomers have the same molecular formula but differ in the connectivity of their atoms. This can lead to significant differences in their physical and chemical properties.

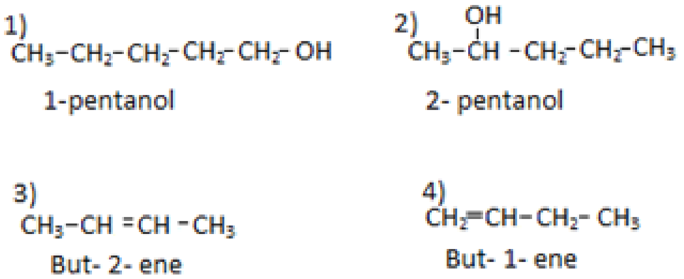
Types of Structural Isomerism:

1. **Chain Isomerism**:
    - **Definition**: Isomers that differ in the arrangement of the carbon skeleton.
    - **Example**: Butane ($CH_3CH_2CH_2CH_3$) and Isobutane ($CH_3CH(CH_3)_2$).

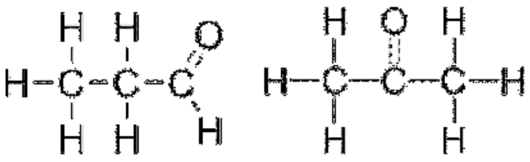


Formulae	IUPAC names
1. $CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$	Hexane
2. $CH_3-CH_2-CH_2-\underset{\underset{CH_3}{\vert}}{CH}-CH_3$	2-methyl pentane
3. $CH_3-CH_2-\underset{\underset{CH_3}{\vert}}{CH}-CH_2-CH_3$	3-methyl pentane
4. $CH_3-CH-\underset{\underset{CH_3}{\vert}}{CH}-\underset{\underset{CH_3}{\vert}}{CH}-CH_3$	2,3-Dimethyl butane
5. $CH_3-CH-\overset{\overset{CH_3}{\vert}}{\underset{\underset{CH_3}{\vert}}{CH}}-CH_2-CH_3$	2,2-Dimethylbutane

2. **Position Isomerism**:
   - **Definition**: Isomers that differ in the position of a functional group or substituent on the carbon chain.
   - **Example**: 1-Propanol ($CH_3CH_2CH_2OH$) and 2-Propanol ($CH_3CHOHCH_3$).



3. **Functional Group Isomerism**:
   - **Definition**: Isomers that differ in the type of functional group present.
   - **Example**: Ethanol (CH_3CH_2OH, an alcohol) and Dimethyl Ether (CH_3OCH_3, an ether).



Propanal (C_3H_6O) Propanone (C_3H_6O)

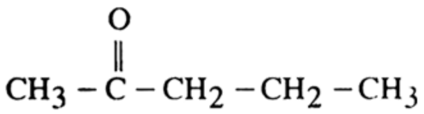
4. **Metamerism**:
   - **Definition**: Isomers that differ in the distribution of alkyl groups on either side of a functional group.
   - **Example**: Ethyl Propyl Ether ($CH_3CH_2OCH_2CH_2CH_3$) and Propyl Ethyl Ether ($CH_3CH_2CH_2OCH_3$).

$$CH_3 - CH_2 - O - CH_2 - CH_3$$

Ethoxyethane

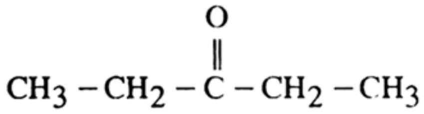
$$CH_3 - O - CH_2 - CH_2 - CH_3$$

1-Methoxypropane



$$CH_3 - \overset{\overset{\displaystyle O}{\|}}{C} - CH_2 - CH_2 - CH_3$$

Pentan-2-one



$$CH_3 - CH_2 - \overset{\overset{\displaystyle O}{\|}}{C} - CH_2 - CH_3$$

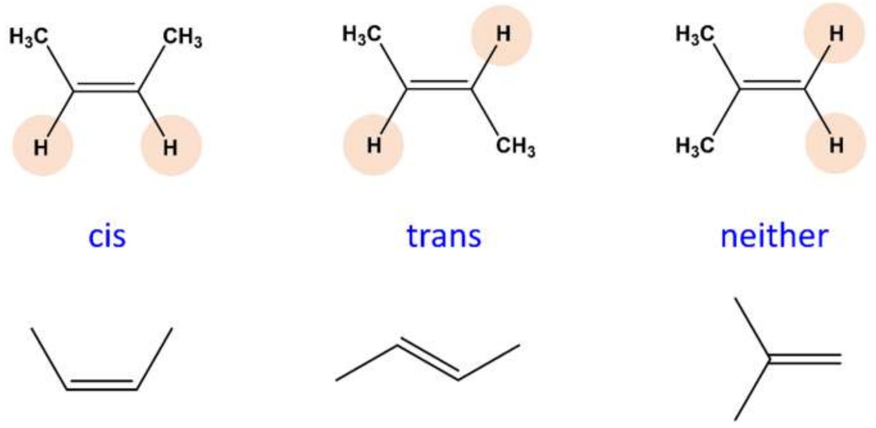
Pentan-3-one

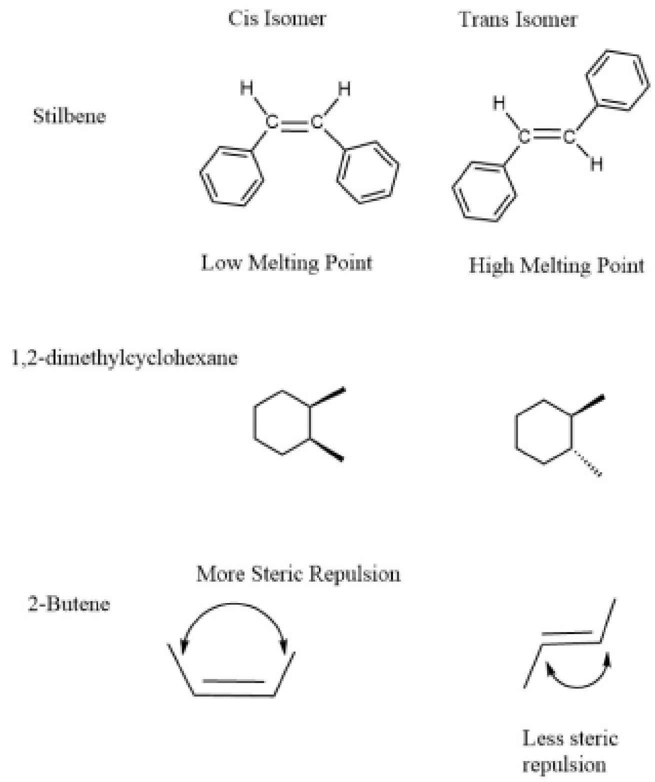
5.2.2 Stereoisomerism

Stereoisomers have the same connectivity of atoms but differ in their spatial arrangement. This can lead to differences in physical and chemical properties, especially in biological systems.

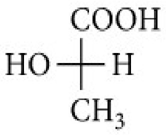
Types of Stereoisomerism:

1. **Geometric (Cis-Trans) Isomerism**:
   - **Definition**: Isomers that differ in the spatial arrangement of groups around a double bond or a ring structure.
   - **Example**: Cis-2-butene ($CH_3CH=CHCH_3$, with both methyl groups on the same side) and Trans-2-butene ($CH_3CH=CHCH_3$, with methyl groups on opposite sides).

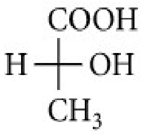




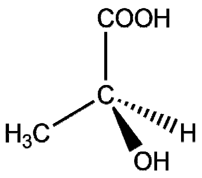
2. **Optical Isomerism**:
   - **Definition**: Isomers that are non-superimposable mirror images of each other, also known as enantiomers.
   - **Example**: Lactic Acid ($CH_3CH(OH)COOH$) exists in two enantiomeric forms, D-lactic acid and L-lactic acid. These forms can rotate plane-polarized light in opposite directions.



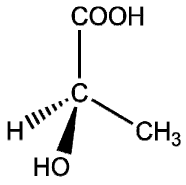
L(+) lactic acid



D(−) lactic acid

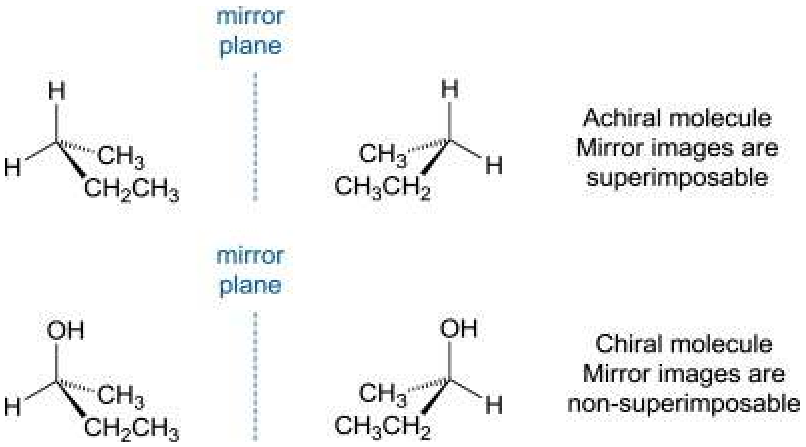


l- lactic acid



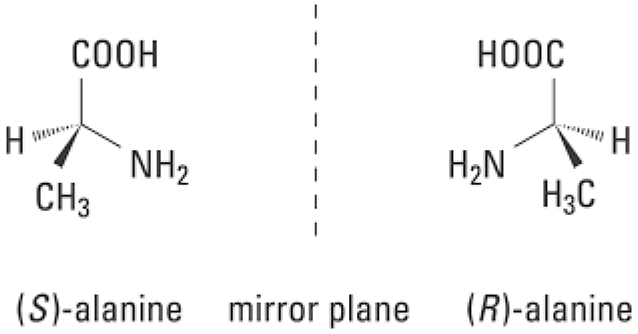
d-lactic acid

Chirality and Chiral Centers:

- **Chiral Center**: A carbon atom that is attached to four different groups. Such a carbon atom is called a chiral center.
- **Example**: In 2-butanol ($CH_3CH(OH)CH_2CH_3$), the second carbon is a chiral center.
- 

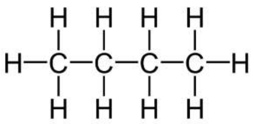
R/S Configuration:

- **Definition**: A system used to describe the absolute configuration of chiral centers. The R/S system assigns a configuration based on the priority of the groups attached to the chiral center.
- **Example**: In 2-butanol, the chiral center can be assigned an R or S configuration based on the spatial arrangement of the groups.

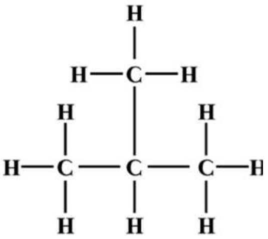


5.3 Examples of Isomers

1. **Butane and Isobutane**:
   - **Molecular Formula**: C_4H_{10}
   - **Structural Isomers**: Butane ($CH_3CH_2CH_2CH_3$) and Isobutane ($CH_3CH(CH_3)_2$).

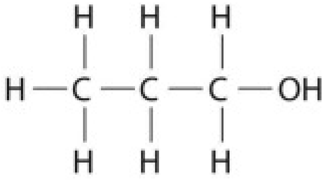


n-butane
or
butane

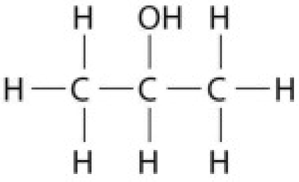


i-butane
or
isobutane

2. **1-Propanol and 2-Propanol**:
   - **Molecular Formula**: C_3H_8O
   - **Position Isomers**: 1-Propanol ($CH_3CH_2CH_2OH$) and 2-Propanol ($CH_3CHOHCH_3$).

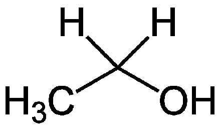


1-Propanol (*n*-propanol)

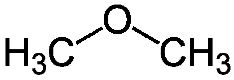


2-Propanol (isopropanol)

3. **Ethanol and Dimethyl Ether**:
   - **Molecular Formula**: C_2H_6O
   - **Functional Group Isomers**: Ethanol (CH_3CH_2OH) and Dimethyl Ether (CH_3OCH_3).

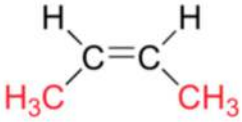


Ethanol (Alcohol)

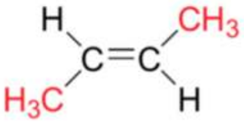


Dimethylether

4. **Cis-2-butene and Trans-2-butene**:
   - **Molecular Formula**: C_4H_8
   - **Geometric Isomers**: Cis-2-butene ($CH_3CH{=}CHCH_3$, cis configuration) and Trans-2-butene ($CH_3CH{=}CHCH_3$, trans configuration).

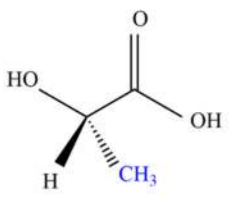


cis-2-butene

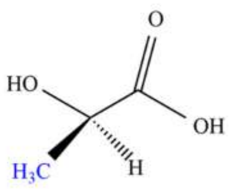


trans-2-butene

5. **D-lactic Acid and L-lactic Acid**:
    - **Molecular Formula**: $C_3H_6O_3$
    - **Optical Isomers**: D-lactic acid and L-lactic acid, which are enantiomers.



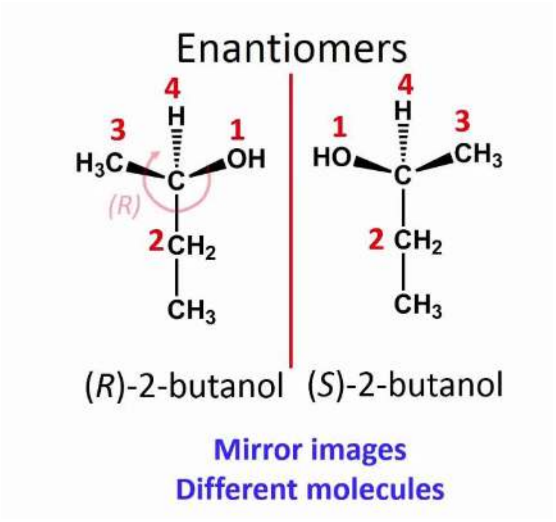
L (+) lactic acid



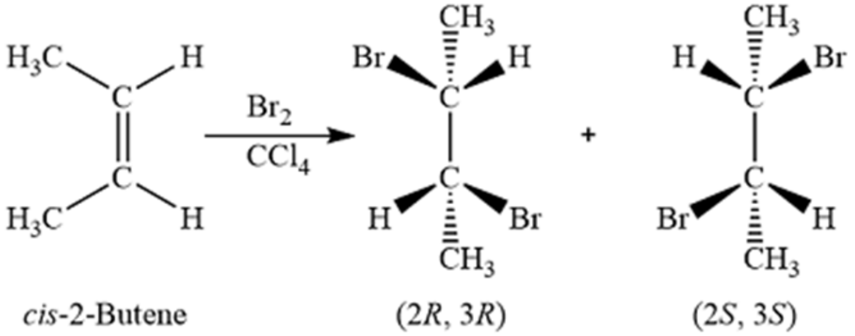
D (-) lactic acid

6- **R/S and E/Z Configurations**

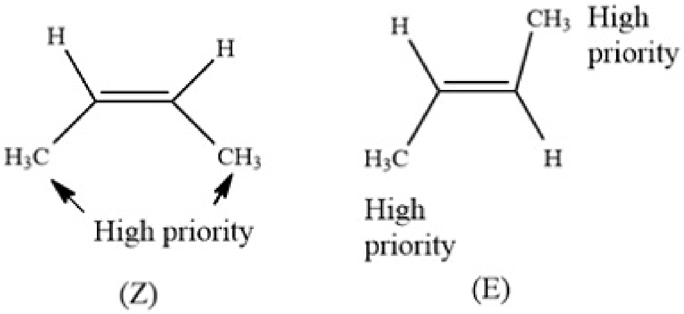
1. **R/S Configuration**
    - **Definition**: The R/S system is used to describe the absolute configuration of chiral centers in molecules.
    - **Example**: (R)-2-butanol and (S)-2-butanol.
    - **Diagram**:



(Note: The (R) and (S) configurations indicate the spatial arrangement of the atoms around the chiral center.)



2. **E/Z Configuration**
   - **Definition**: The E/Z system is used to describe the configuration of double bonds in molecules.
   - **Example**: (E)-2-butene and (Z)-2-butene.
   - **Diagram**:



(Note: The (E) configuration indicates that the higher priority groups are on opposite sides of the double bond, while the (Z) configuration indicates that they are on the same side.)

Electronic effects in organic chemistry play a crucial role in understanding the behavior and reactivity of organic molecules. Here is a detailed explanation of the main electronic effects, including inductive effect, resonance effect, hyperconjugation, and electromeric effect, along with examples and diagrams.

1. Inductive Effect

The inductive effect is a permanent electronic effect that occurs due to the electronegativity difference between atoms in a molecule. It involves the shift of electron density along a chain of atoms through sigma bonds. The effect diminishes with increasing distance from the influencing group

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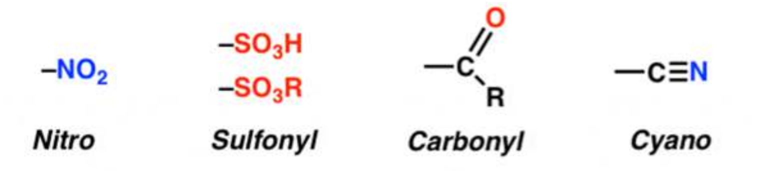
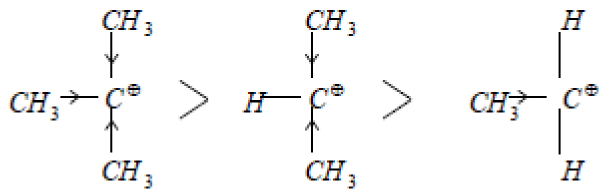
- **Electron-Withdrawing Groups (-I Effect)**: These groups withdraw electron density from the rest of the molecule. Examples include halogens (F, Cl, Br, I) and nitro groups (-NO2).



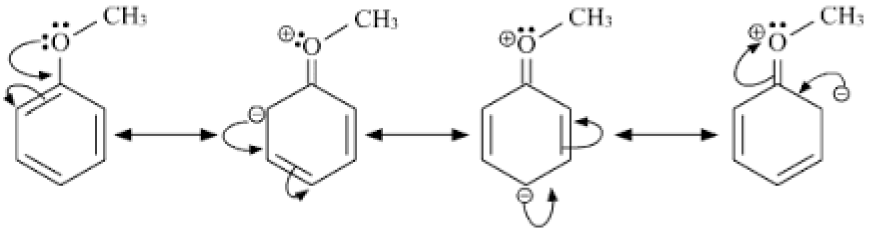
- **Electron-Releasing Groups (+I Effect)**: These groups release electron density towards the rest of the molecule. Examples include alkyl groups (CH3-, C2H5-).



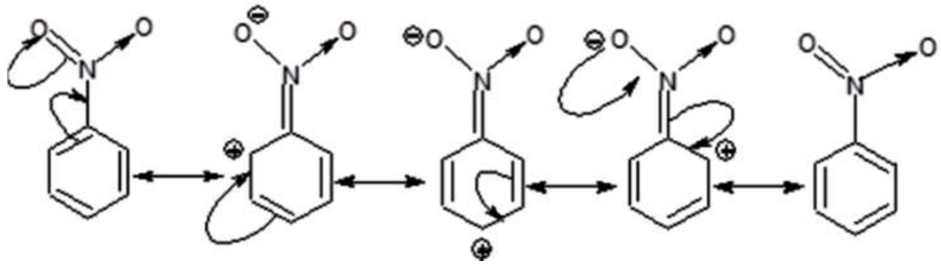
2. Resonance Effect

The resonance effect, also known as the mesomeric effect, involves the delocalization of π-electrons within a molecule. This effect is represented by multiple resonance structures and is crucial for understanding the stability of molecules

- **Positive Resonance Effect (+R Effect)**: This occurs when a substituent donates electron density to the rest of the molecule through π-bonds. Examples include -OH, -OR, and -NH_2 groups.

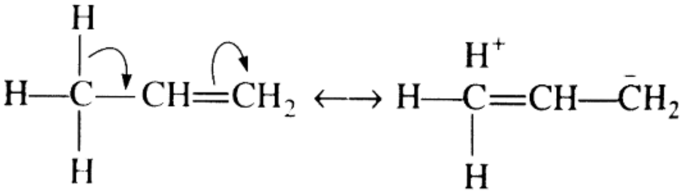


- **Negative Resonance Effect (-R Effect)**: This occurs when a substituent withdraws electron density from the rest of the molecule through π-bonds. Examples include -NO_2, -COOH, and -CN groups.



3. Hyperconjugation

Hyperconjugation involves the delocalization of σ-electrons from C-H bonds to an adjacent empty or partially filled p-orbital or π-system. This effect stabilizes carbocations, alkenes, and free radicals



$$H{-}\overset{H}{\underset{H}{C}}{-}CH{=}CH_2 \longleftrightarrow H{-}\overset{H^+}{\underset{H}{C}}{=}CH{-}\overset{-}{C}H_2$$

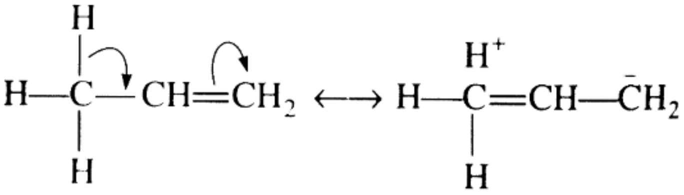
In propene, the C-H σ-bond of the methyl group can overlap with the π-bond of the alkene, stabilizing the molecule

4. Electromeric Effect

The electromeric effect is a temporary effect that occurs in the presence of an attacking reagent. It involves the complete transfer of a shared pair of π-electrons to one of the atoms in a multiple bond

- **Positive Electromeric Effect (+E Effect)**: The π-electrons are transferred towards the attacking reagent.
- **Negative Electromeric Effect (-E Effect)**: The π-electrons are transferred away from the attacking reagent.

Diagram:



$$H{-}\overset{H}{\underset{H}{C}}{-}CH{=}CH_2 \longleftrightarrow H{-}\overset{H^+}{\underset{H}{C}}{=}CH{-}\overset{-}{C}H_2$$

In this example, the π-electrons are transferred towards the attacking proton (H^+), resulting in the formation of a carbocation

These electronic effects are fundamental to understanding the behavior of organic molecules and predicting their reactivity. Each effect has a unique impact on the stability and reactivity of molecules, making them essential concepts in organic chemistry.

Mesomeric Effect in Organic Chemistry

The mesomeric effect, also known as the resonance effect, is a fundamental concept in organic chemistry that describes the delocalization of π-electrons within a molecule. This effect significantly influences the stability, reactivity, acidity, and basicity of organic compounds. Here’s a detailed explanation with examples and diagrams.

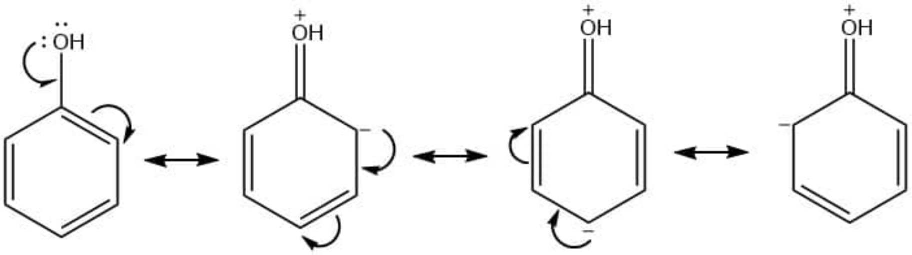
Definition and Types

The mesomeric effect occurs when π-electrons or lone pairs of electrons are delocalized across a conjugated system. This delocalization can stabilize or destabilize molecules, depending on the nature of the substituents.

- **Positive Mesomeric Effect (+M Effect)**: This occurs when a substituent donates electron density to the conjugated system, stabilizing it. Examples include -OH, -OR, -NH2, and -SH groups.
- **Negative Mesomeric Effect (-M Effect)**: This occurs when a substituent withdraws electron density from the conjugated system, destabilizing it. Examples include -NO2, -COOH, -CN, and -C=O groups.

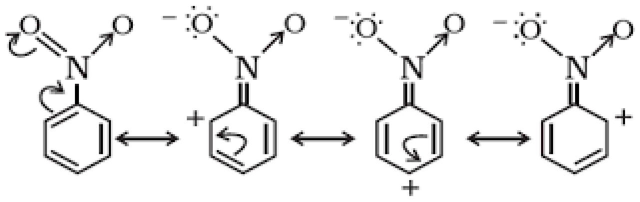
Examples and Diagrams

1. Positive Mesomeric Effect (+M Effect)
Consider the example of phenol (C_6H_5OH). The hydroxyl group (-OH) donates electron density to the benzene ring through resonance, stabilizing the molecule.
Resonance Structures of Phenol:



In the resonance structures, the lone pair on the oxygen atom of the hydroxyl group can delocalize into the benzene ring, creating a more stable structure

2. Negative Mesomeric Effect (-M Effect)
Consider nitrobenzene ($C_6H_5NO_2$). The nitro group ($-NO_2$) withdraws electron density from the benzene ring through resonance, destabilizing the molecule.
Resonance Structures of Nitrobenzene:
In the resonance structures, the nitro group withdraws electron density from the benzene ring, creating a less stable structure



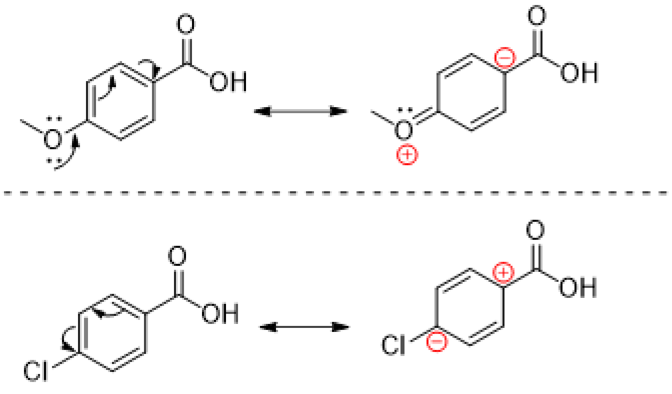
Impact on Acidity and Basicity

The mesomeric effect significantly influences the acidity and basicity of organic compounds by altering the electron density around the functional groups.

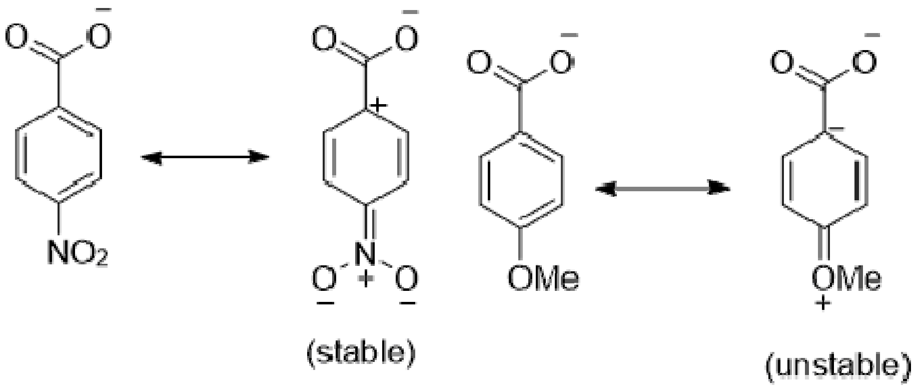
- **Acidity**: Electron-donating groups (e.g., -OH, -OR) increase the electron density in the carbonyl group, reducing acidity. Electron-withdrawing groups (e.g., $-NO_2$, -COOH) decrease electron density, increasing acidity.
- **Basicity**: Electron-donating groups (e.g., $-NH_2$) increase basicity by stabilizing the positive charge. Electron-withdrawing groups (e.g., -C=O) decrease basicity by withdrawing electron density

Example:

- **Para-methoxybenzoic acid (p-MeO-C_6H_4-COOH)**: The methoxy group ($-OCH_3$) donates electron density to the carboxyl group, reducing its acidity compared to benzoic acid



- **Para-nitrobenzoic acid (p-NO_2-C_6H_4-COOH)**: The nitro group ($-NO_2$) withdraws electron density from the carboxyl group, increasing its acidity compared to benzoic acid



Effects on Nucleophilic and Electrophilic Reactions

The mesomeric effect also influences nucleophilic and electrophilic reactions by altering the electron density distribution.

- **Nucleophilic Reactions**: Electron-donating groups increase nucleophilicity by donating electron density. Electron-withdrawing groups decrease nucleophilicity by withdrawing electron density
- **Electrophilic Reactions**: Electron-donating groups enhance electrophilicity by increasing electron density on the electrophilic center. Electron-withdrawing groups decrease electrophilicity by withdrawing electron density

Conclusion

The mesomeric effect is a crucial concept in organic chemistry that helps explain the stability, reactivity, acidity, and basicity of organic compounds. Understanding this effect is essential for predicting and controlling the outcomes of organic reactions. By manipulating the mesomeric effect, chemists can design more efficient and selective reactions

5.4 Importance of Isomerism

Isomerism is crucial in understanding the behavior of organic compounds. Structural isomers can have vastly different properties, while stereoisomers can have subtle differences that are significant in biological contexts. For example, the effectiveness of a drug can depend on its stereochemistry, as different enantiomers can have different biological activities.

5.5 Conclusion

Isomerism is a fundamental concept in organic chemistry that highlights the importance of molecular structure and spatial arrangement. Understanding isomerism helps in predicting the properties and reactivities of organic compounds, which is essential in fields such as pharmaceuticals, materials science, and biochemistry.

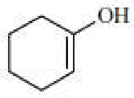
Exercise 1

1. Provide some functional isomers corresponding to the molecular formula $C_6H_{12}O_2$.
2. Provide all positional and skeletal isomers of acids corresponding to this formula.

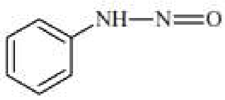
Exercise 2

Provide the tautomeric forms corresponding to the following compounds:

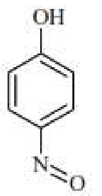
1°



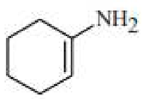
2°



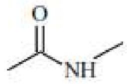
3°



4°



5°



Exercise 3

Consider the compound with the formula CH_3-$CH(NHCH_3)$-$CHOH$-C_6H_5.

1. Provide the Fischer representation of all stereoisomers of this compound.
2. Provide the absolute configurations of the asymmetric carbons.
3. Provide the Newman representation of a stable conformer of this compound with the absolute configuration RR.

Exercise 4

Consider the carboxylic acids with the molecular formula $C_4H_6Br_2O_2$ (limited to compounds that do not have both bromine atoms on the same carbon).

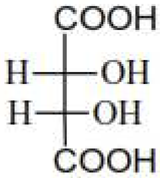
1. Write the expanded formula of possible isomers and for each, specify which carbon atoms are asymmetric.
2. Among these isomers, only one has two asymmetric carbon atoms;

   Represent these stereoisomers in Cram, Newman, and Fischer projections.

Specify their stereochemical relationships and give the absolute configuration of each asymmetric carbon.

Exercise 5

I. Consider one of the stereoisomers of tartaric acid whose Fischer representation is as follows:

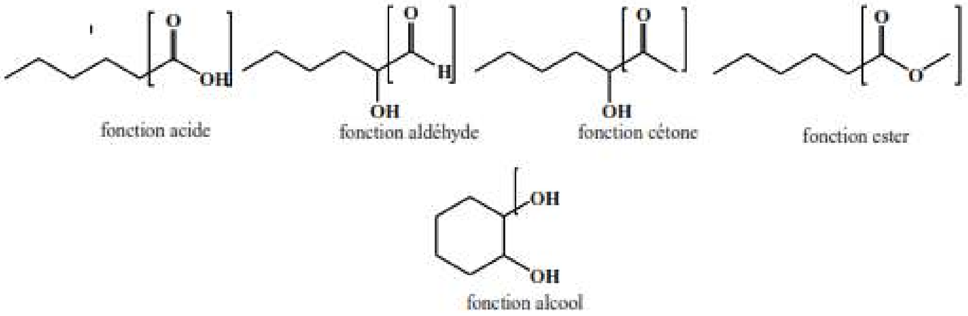


I-1. Provide the systematic name of this compound.
I-2. Specify the absolute configuration of each asymmetric carbon.
I-3. Is this compound chiral?
II. (+)-Tartaric acid is of absolute configuration 2R, 3R.
II-1. Represent it in Fischer projection. Is it chiral?
II-2. Specify its D or L series.
II-3. Represent its enantiomer in Fischer projection, specifying its absolute configuration, D or L series, and the sign of its specific rotation.

Solutions

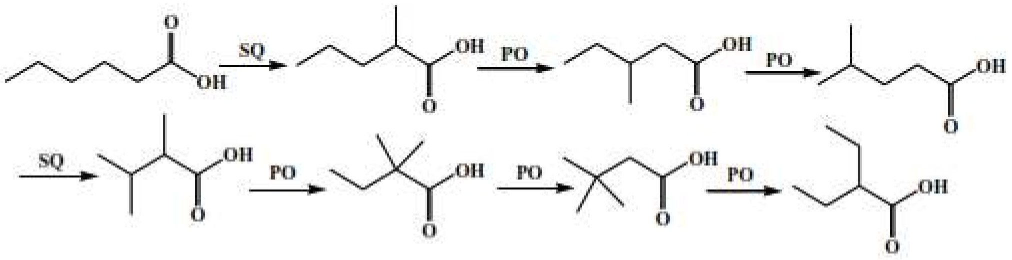
Exercise 1

1. Calculate the degree of unsaturation: $(C_6H_{12}O_2)$/Ni = 6 - 12/2 + 1 = 1. Ni = 1 means the compound includes either a double bond or a cycle. Therefore, the 5 isomers are as follows:



fonction acide
fonction aldéhyde
fonction cétone
fonction ester
fonction alcool

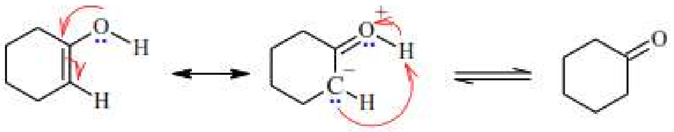
2. Skeletal (SQ) and positional (PO) isomers of acids corresponding to this formula are as follows:



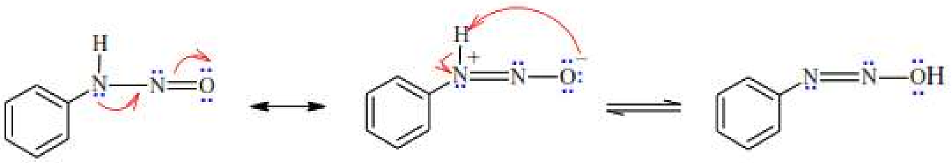
Exercise 2

Determination of tautomeric forms:

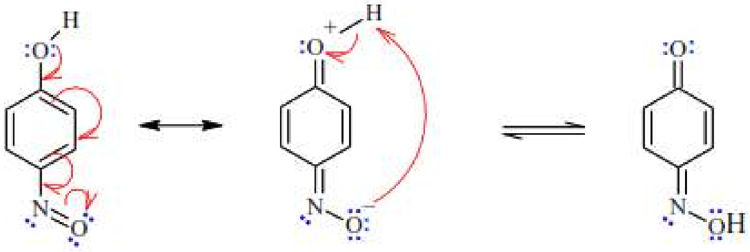
1°



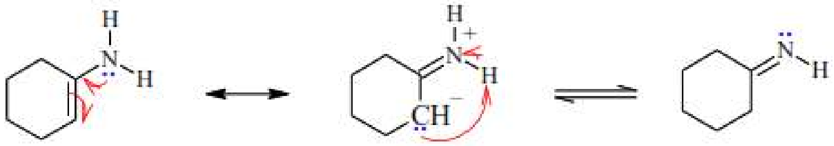
2°



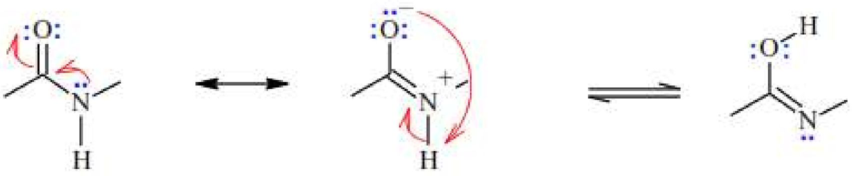
3°



4°



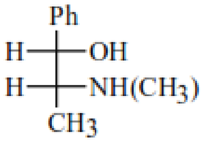
5°



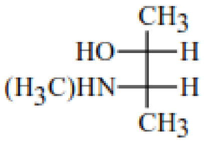
function acid function aldehyde function ketone function ester
function alcohol

Exercise 3

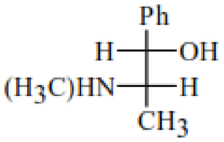
Q1, Q2



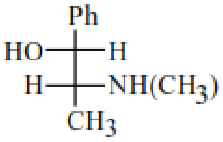
(S, R)



(R, S)

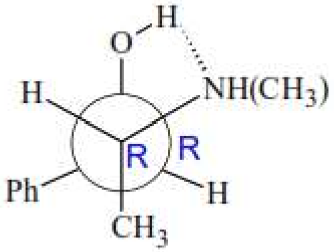


(S, S)



(R, R)

3. The Newman representation of a stable conformer:



R R (Intramolecular hydrogen bond)

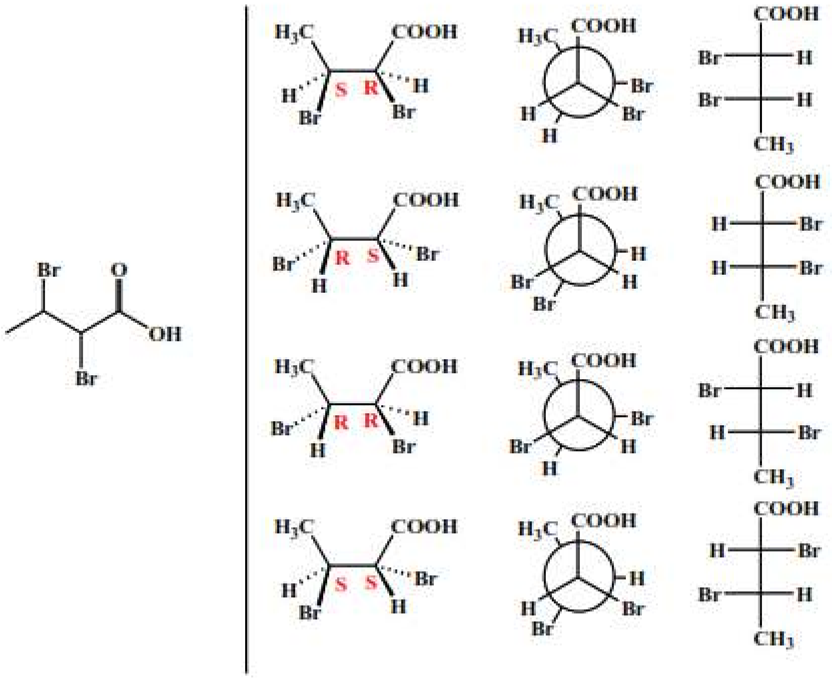
This conformer is stable due to the presence of an intramolecular hydrogen bond between the -OH and NH(CH_3) groups (it has a stabilizing effect).

Exercise 4

1/ Ni= 1

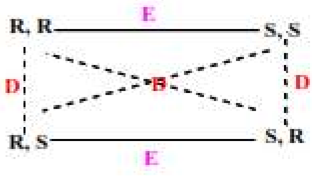
2/ The number of stereoisomers is: $2^n = 4$ (n represents the number of asymmetric carbons)

a- Representation of stereoisomers in Cram, Newman, and Fischer projections.



- (S, R) and (R, S) are erythro: the two -Br groups appear on the same side of the bond between the two chiral centers.
- (R, R) and (S, S) are threo: the two -Br groups appear on opposite sides of the bond between the two chiral centers.

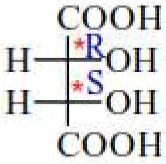
b- The following diagram reveals the relationship between these stereoisomers:



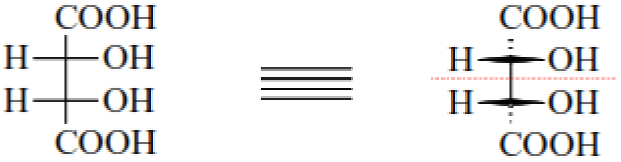
E: enantiomers
D: diastereomers

Exercise 5

I. 2,3-Dihydroxybutane-1,4-dioic acid.
I-2

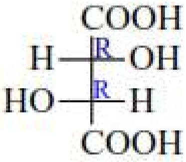


I-3 It is noted that the molecule has a plane of symmetry, making it achiral (it is a meso form).



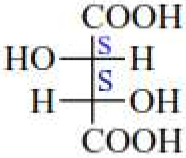
Plane of symmetry

II-1, II-2



It is noted that there is no longer a plane of symmetry, which makes the molecule chiral.
On the last asymmetric carbon, the -OH group is on the left, so it belongs to the L series.

II-3

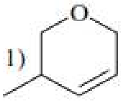


On the last asymmetric carbon, the -OH group is on the right, so it belongs to the D series.
This enantiomer is levorotatory (-)
The specific rotations of enantiomers are opposite.

Supplementary Exercise

Exercise 1:

1. Give the hybridization state of the carbon atoms in the following compounds:

1) 

2) 

3) 

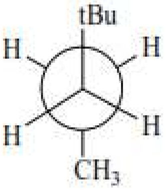
$CH_2{=}CH{-}CH_2{-}CH{=}C{=}CH{-}CH_3$

4) 

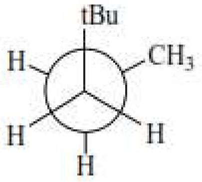
2. Write all the planar isomers corresponding to the molecular formulas: C_3H_9N, C_4H_8O, $C_5H_{10}O$
3. What is the geometry of the following molecules: $CHCl_3$, $C_2H_2Cl_2$, $CH{\equiv}CH$, $CH_2{=}C{=}CH_2$

Exercise 2:

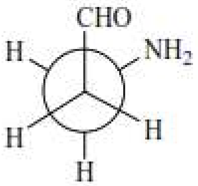
1. Compare the stability of the following conformers:



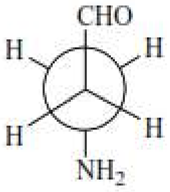
Et



,



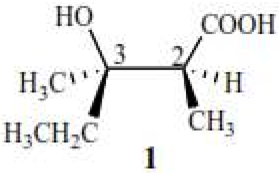
Et



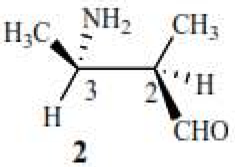
2. Draw approximately the curve $Ep = f(\theta)$ for 2-Fluoropropanol

Exercise 3:

1. Represent molecules 1 and 2 according to Newman along the C2-C3 axis, keeping the proposed conformations:



1



2

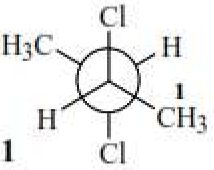
2. Represent molecules 1 and 2 according to Fischer

Exercise 4:

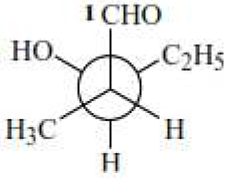
1. From the spatial geometry of cyclohexane, which we will specify, give the possible isomers of the various dichlorocyclohexanes.
2. Which isomer is the most stable for each of the following pairs:
    - 3-5-dimethyl-1-chlorocyclohexane (e,a,a) and (a,a,a)
    - 2-tertiobutylcyclohexanol (e,e) and (a,a)
    - Cyclohexan-1,2-diol (e,e) and (a,a).

Exercise 5:

1. Represent the following molecules according to Fischer, positioning carbon 1 at the top:

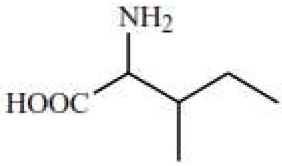


1

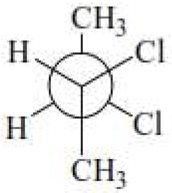


2

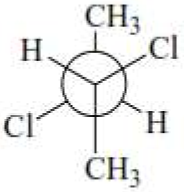
2. Represent in perspective, in Fischer projection all possible stereoisomers of isoleucine



Exercise 6: Indicate whether the following molecules are conformers, enantiomers, or diastereomers. The absolute configuration of the carbons will be indicated for each molecule.



1



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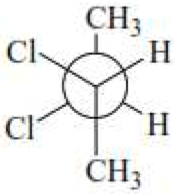

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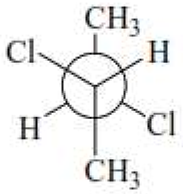
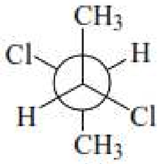
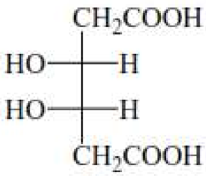


4

Exercise 7:

1. Indicate whether each of the following molecules is chiral or not. Justify your answer.


1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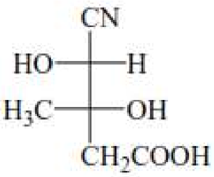
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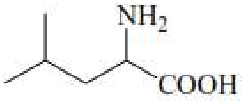
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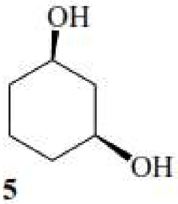
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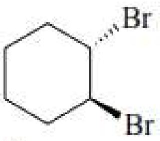
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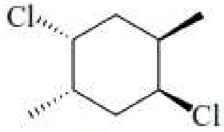
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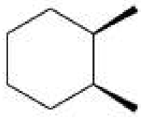
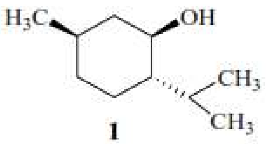

8

Exercise 8:

1. What type of isomerism exists between the following 3 molecules 1, 2, and 3?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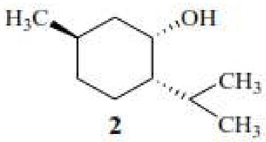
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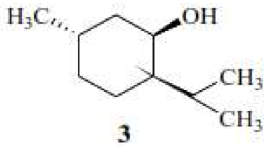
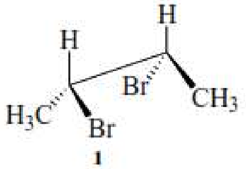

3

2. Provide the Cram perspective representations and Newman projections of the configurations of 3-chloro-2-hydroxybutanoic acid: (2S, 3S) and (2R, 3S)
3. Write the structure of:
    - a) (E)-penta-1,3-diene
    - b) (2E,4Z,7Z)-7-bromo-4-ethyl-8-methyldec-2,4,7-triene.

Exercise 9: Identify among the structures below the forms Méso, Erythro, and Thréo.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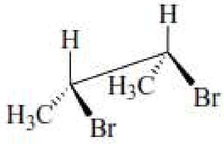
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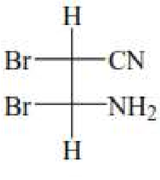
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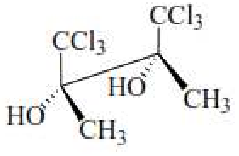
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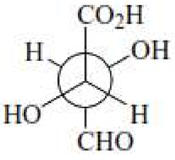
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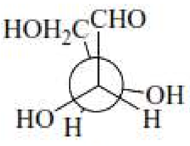
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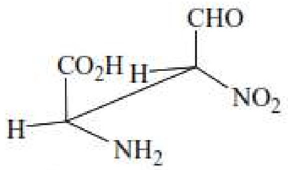
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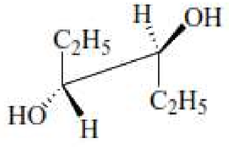
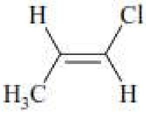
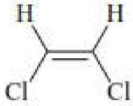
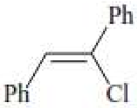
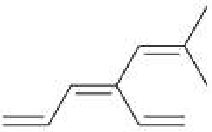

8

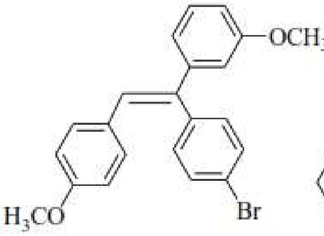
Exercise 10: Determine the Z or E, Cis or Trans configuration of the following molecules:

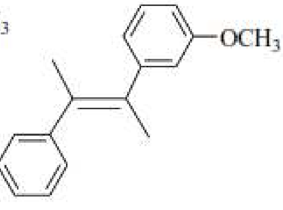

H
Cl
H_3C
H

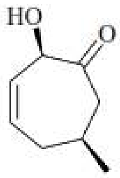

H
H
Cl
Cl

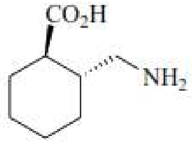

Ph
Ph
Cl

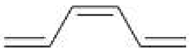



OCH_3
H_3CO
Br


OCH_3


HO
O


CO_2H
NH_2



Chapter 6: Stereochemistry

6.1 Chirality

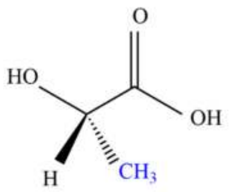
Chiral molecules have a non-superimposable mirror image, known as enantiomers.

6.2 Optical Activity

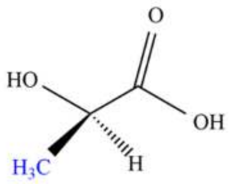
Chiral molecules can rotate plane-polarized light, a property known as optical activity.

Example: Lactic Acid

Lactic acid ($CH_3CH(OH)COOH$) exists in two enantiomeric forms, D-lactic acid and L-lactic acid.



L (+) lactic acid



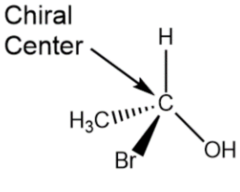
D (-) lactic acid

Chapter 6: Stereochemistry

6.1 Chirality

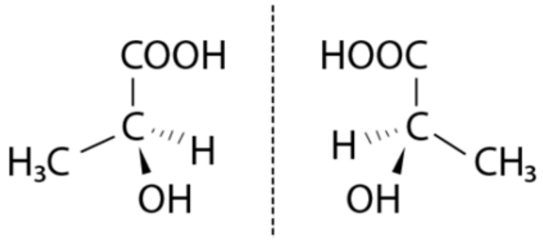
Definition: Chirality refers to the property of molecules that have a non-superimposable mirror image. These molecules are known as chiral molecules, and their non-superimposable mirror images are called enantiomers.
Chiral Centers:

- **Definition**: A chiral center is a carbon atom (or any other atom) that is attached to four different groups. Such a carbon atom is also called an asymmetric carbon.
- **Example**: In 2-butanol ($CH_3CH(OH)CH_2CH_3$), the second carbon atom is a chiral center because it is attached to four different groups: a methyl group (CH_3), a hydrogen atom (H), a hydroxyl group (OH), and an ethyl group (CH_2CH_3).

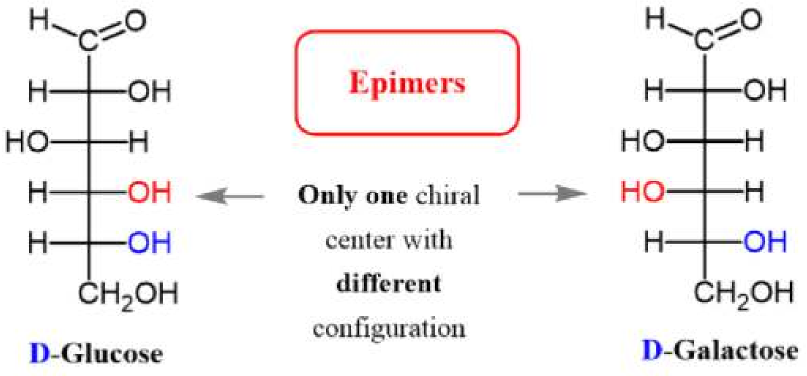


Enantiomers:

- **Definition**: Enantiomers are pairs of chiral molecules that are non-superimposable mirror images of each other. They have the same molecular formula and the same connectivity of atoms but differ in their spatial arrangement.
- **Example**: Lactic acid ($CH_3CH(OH)COOH$) exists in two enantiomeric forms: D-lactic acid and L-lactic acid. These forms are non-superimposable mirror images of each other.



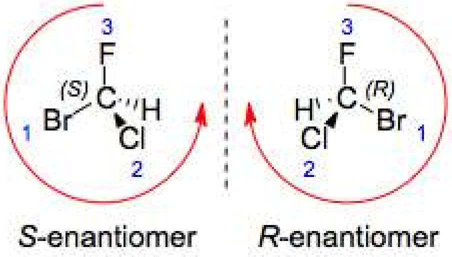
D-glucose and D-galactose are epimeric at carbon-4

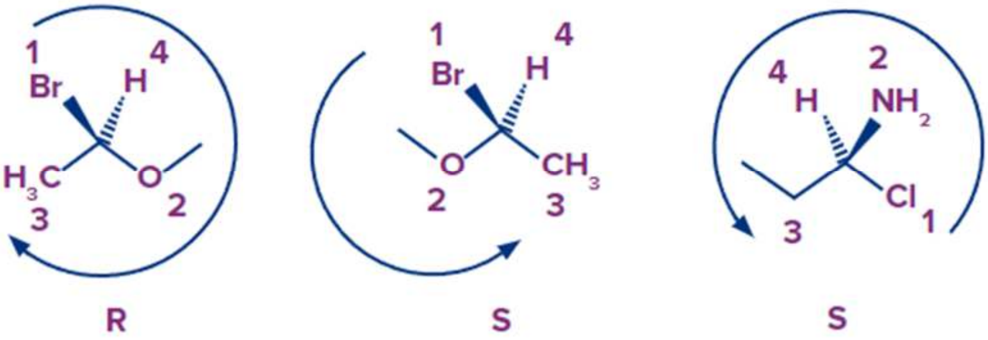


R/S Configuration:

- **Definition**: The R/S system is used to describe the absolute configuration of chiral centers. The configuration is assigned based on the priority of the groups attached to the chiral center.
- **Priority Rules**: The groups attached to the chiral center are ranked according to their atomic numbers. The highest atomic number gets the highest priority.
  1. **First Priority**: The group with the highest atomic number.
  2. **Second Priority**: The next highest atomic number.
  3. **Third Priority**: The next highest atomic number.
  4. **Fourth Priority**: The lowest atomic number.

- **Assigning Configuration**:
  - If the priority order of the groups goes clockwise when viewed from the fourth priority group, the configuration is R (rectus).
  - If the priority order of the groups goes counterclockwise when viewed from the fourth priority group, the configuration is S (sinister).





Example: In 2-butanol ($CH_3CH(OH)CH_2CH_3$), the chiral center can be assigned an R or S configuration based on the spatial arrangement of the groups.

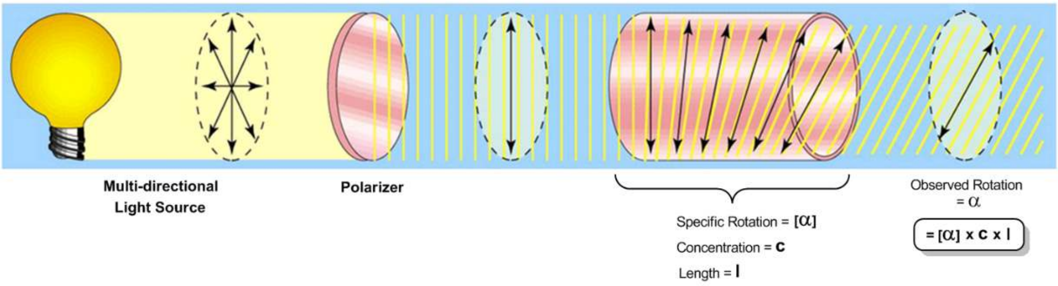
6.2 Optical Activity

Definition: Optical activity is the ability of chiral molecules to rotate plane-polarized light. This property arises because chiral molecules interact differently with left- and right-handed plane-polarized light.
Plane-Polarized Light:

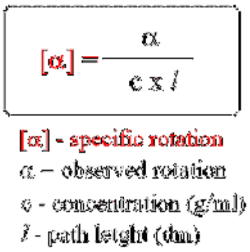
- **Definition**: Light that vibrates in a single plane.
- **Polarimeter**: An instrument used to measure the rotation of plane-polarized light.

Specific Rotation:

- **Definition**: The specific rotation of a chiral compound is the angle through which plane-polarized light is rotated by a standard solution of the compound.

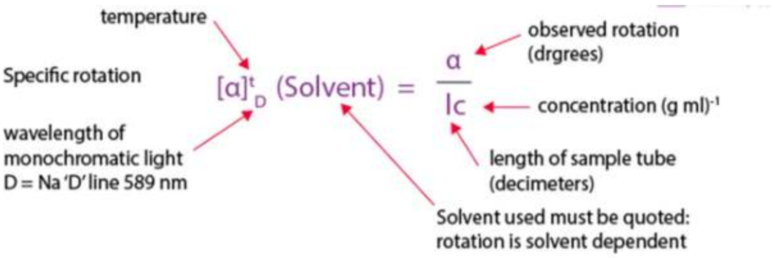


- **Units**: Specific rotation is measured in degrees per decimeter per gram per milliliter (°/dm/g/mL).



$$[\alpha] = \frac{\alpha}{c \times l}$$

[α] - specific rotation
α – observed rotation
c - concentration (g/ml)
l - path letght (dm)

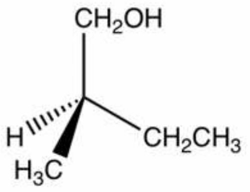


Enantiomers and Optical Activity:

- **Dextrorotatory (D) Enantiomers**: Rotate plane-polarized light to the right (+).
- **Levorotatory (L) Enantiomers**: Rotate plane-polarized light to the left (-).

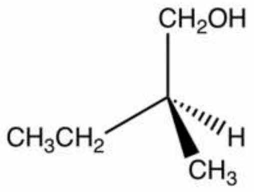
Example: Lactic acid exists in two enantiomeric forms:

- **D-lactic acid**: Rotates plane-polarized light to the right (+).
- **L-lactic acid**: Rotates plane-polarized light to the left (-).



(R)-2-methyl-1-butnaol

$[\alpha]_D^{20°C} = +5.75°$



(S)-2-methyl-1-butnaol

$[\alpha]_D^{20°C} = -5.75°$

Racemic Mixtures:

- **Definition**: A racemic mixture is a 1:1 mixture of two enantiomers. Racemic mixtures do not rotate plane-polarized light because the rotations caused by the two enantiomers cancel each other out.
- **Example**: A racemic mixture of D-lactic acid and L-lactic acid will not show any net rotation of plane-polarized light.

6.3 Importance of Chirality and Optical Activity

Biological Significance:

- **Enantioselectivity**: Biological systems often recognize and respond differently to enantiomers. For example, one enantiomer of a drug may be effective, while the other may be inactive or even harmful.
- **Example**: Thalidomide, a drug used in the 1950s, had one enantiomer that was effective against morning sickness, while the other enantiomer caused severe birth defects.

Applications in Chemistry:

- **Chiral Synthesis**: Chemists often aim to synthesize chiral compounds in a specific enantiomeric form to ensure the desired biological activity.
- **Chiral Catalysts**: Catalysts that can selectively produce one enantiomer over another are crucial in the synthesis of chiral compounds.

6.4 Conclusion

Stereochemistry, particularly chirality and optical activity, is a fundamental aspect of organic chemistry. Understanding these concepts is crucial for predicting the behavior of chiral compounds in various chemical and biological contexts. The ability to distinguish between enantiomers and control their synthesis is essential in fields such as pharmaceuticals, agrochemicals, and materials science.

Chapter 7: Acids and Bases in Organic Chemistry

7.1 Acids and Bases

Organic acids and bases play a crucial role in many chemical reactions.

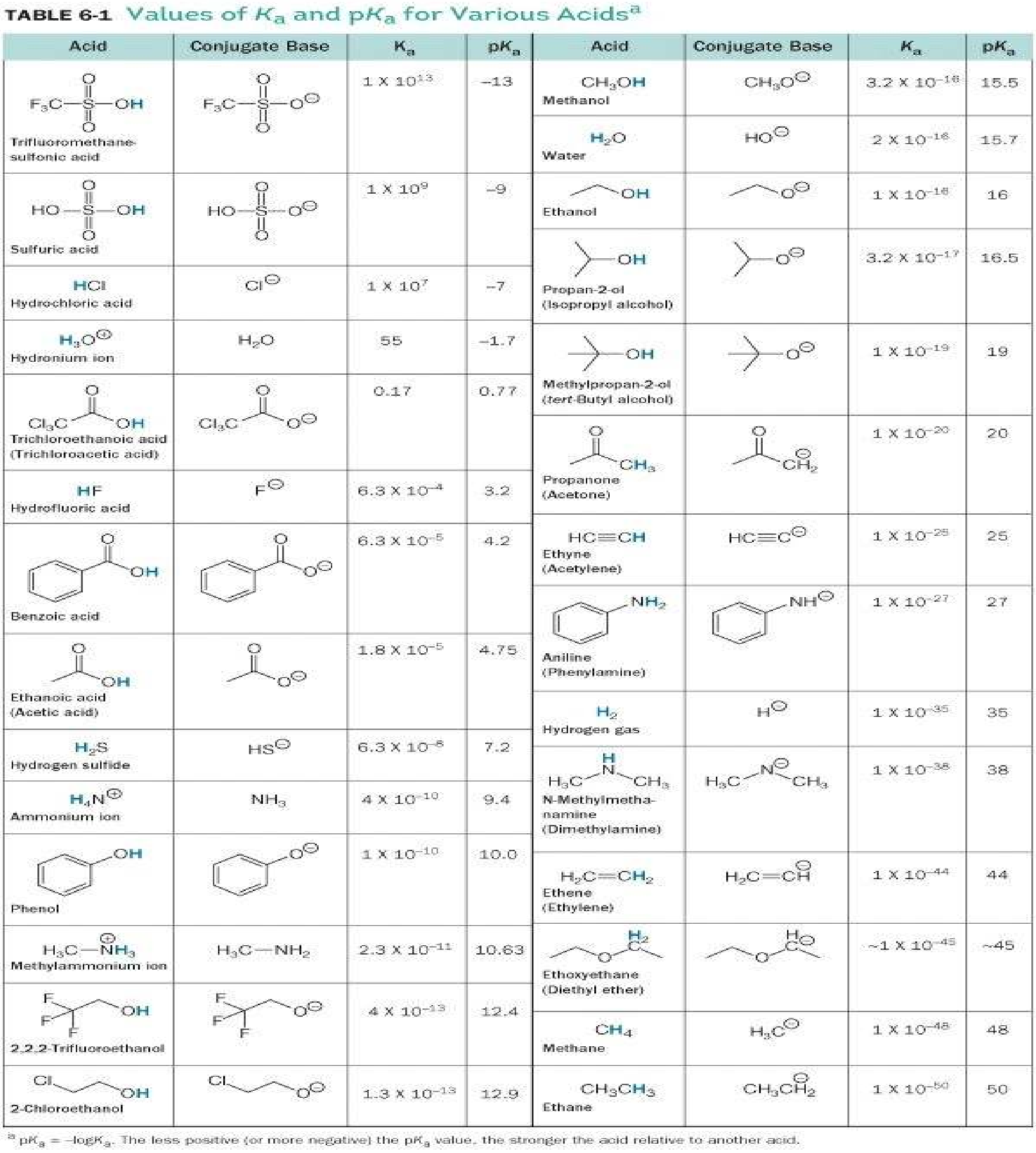
7.2 pKa Values

The pKa value indicates the strength of an acid. Lower pKa values represent stronger acids.

Example: Acetic Acid (CH_3COOH)

Acetic acid is a weak organic acid with a pKa of 4.76.

TABLE 6-1 Values of K_a and pK_a for Various Acids[a]



Acid	Conjugate Base	K_a	pK_a
Trifluoromethanesulfonic acid		1×10^{13}	−13
Sulfuric acid		1×10^{9}	−9
HCl Hydrochloric acid	$Cl^{\ominus}$	1×10^{7}	−7
$H_3O^{\oplus}$ Hydronium ion	H_2O	55	−1.7
Trichloroethanoic acid (Trichloroacetic acid)		0.17	0.77
HF Hydrofluoric acid	$F^{\ominus}$	6.3×10^{-4}	3.2
Benzoic acid		6.3×10^{-5}	4.2
Ethanoic acid (Acetic acid)		1.8×10^{-5}	4.75
H_2S Hydrogen sulfide	$HS^{\ominus}$	6.3×10^{-8}	7.2
$H_4N^{\oplus}$ Ammonium ion	NH_3	4×10^{-10}	9.4
Phenol		1×10^{-10}	10.0
$H_3C-\overset{\oplus}{N}H_3$ Methylammonium ion	H_3C-NH_2	2.3×10^{-11}	10.63
2,2,2-Trifluoroethanol		4×10^{-13}	12.4
2-Chloroethanol		1.3×10^{-13}	12.9

Acid	Conjugate Base	K_a	pK_a
CH_3OH Methanol	$CH_3O^{\ominus}$	3.2×10^{-16}	15.5
H_2O Water	$HO^{\ominus}$	2×10^{-16}	15.7
Ethanol		1×10^{-16}	16
Propan-2-ol (Isopropyl alcohol)		3.2×10^{-17}	16.5
Methylpropan-2-ol (*tert*-Butyl alcohol)		1×10^{-19}	19
Propanone (Acetone)		1×10^{-20}	20
$HC\equiv CH$ Ethyne (Acetylene)	$HC\equiv C^{\ominus}$	1×10^{-25}	25
Aniline (Phenylamine)		1×10^{-27}	27
H_2 Hydrogen gas	$H^{\ominus}$	1×10^{-35}	35
N-Methylmethanamine (Dimethylamine)		1×10^{-38}	38
$H_2C=CH_2$ Ethene (Ethylene)	$H_2C=\overset{\ominus}{C}H$	1×10^{-44}	44
Ethoxyethane (Diethyl ether)		$\sim 1 \times 10^{-45}$	~45
CH_4 Methane	$H_3C^{\ominus}$	1×10^{-48}	48
CH_3CH_3 Ethane	$CH_3\overset{\ominus}{C}H_2$	1×10^{-50}	50

[a] $pK_a = -\log K_a$. The less positive (or more negative) the pK_a value, the stronger the acid relative to another acid.

Chapter 7: Acids and Bases in Organic Chemistry

7.1 Acids and Bases

Definition: Organic acids and bases are fundamental to many chemical reactions in organic chemistry. They play crucial roles in determining the reactivity and stability of organic compounds.

Acids:

- **Definition**: An acid is a substance that donates a proton (H^+) in a chemical reaction.
- **Examples**: Carboxylic acids (R-COOH), phenols (Ar-OH), and sulfonic acids ($R\text{-}SO_3H$).

Bases:

- **Definition**: A base is a substance that accepts a proton (H^+) in a chemical reaction.
- **Examples**: Amines ($R\text{-}NH_2$), alcohols (R-OH), and alkoxides ($R\text{-}O^-$).

Acid-Base Reactions:

- **General Reaction**: An acid donates a proton to a base, forming a conjugate base and a conjugate acid.

Acid+Base→Conjugate Base+Conjugate Acid

- **Example**: The reaction between acetic acid (CH_3COOH) and ammonia (NH_3):

CH3COOH+NH3→CH3COO−+NH4+

7.2 pKa Values

Definition: The pKa value is a measure of the strength of an acid. It is defined as the negative logarithm of the acid dissociation constant (Ka).

pKa=−log(Ka)

Significance:

- **Lower pKa Values**: Represent stronger acids. A lower pKa value indicates that the acid dissociates more readily, releasing H^+ ions more easily.
- **Higher pKa Values**: Represent weaker acids. A higher pKa value indicates that the acid dissociates less readily, releasing H^+ ions less easily.

Examples:

- **Acetic Acid (CH_3COOH)**: pKa ≈ 4.76

  - Acetic acid is a weak acid, meaning it does not dissociate completely in water.
- **Hydrochloric Acid (HCl)**: pKa ≈ -6
  - Hydrochloric acid is a strong acid, meaning it dissociates completely in water, releasing H^+ ions readily.
- **Phenol (C_6H_5OH)**: pKa ≈ 10
  - Phenol is a weak acid, less acidic than acetic acid.

Factors Affecting pKa Values:

1. **Electronegativity**:
   - **Higher Electronegativity**: Atoms that are more electronegative (e.g., oxygen, nitrogen) can stabilize the negative charge on the conjugate base, making the acid stronger.
   - **Example**: Carboxylic acids (R-COOH) are stronger acids than alcohols (R-OH) because the carboxylate ion ($R\text{-}COO^-$) is more stabilized by resonance.
2. **Resonance Stabilization**:
   - **Resonance Structures**: The presence of resonance structures can stabilize the conjugate base, making the acid stronger.
   - **Example**: The conjugate base of acetic acid (CH_3COO^-) is stabilized by resonance, making acetic acid a stronger acid than ethanol (CH_3CH_2OH).
3. **Inductive Effects**:
   - **Electron-Withdrawing Groups**: Groups that withdraw electron density (e.g., $-NO_2$, -Cl) can stabilize the negative charge on the conjugate base, making the acid stronger.
   - **Example**: Trifluoroacetic acid (CF_3COOH) is a stronger acid than acetic acid (CH_3COOH) due to the electron-withdrawing effect of the trifluoromethyl group (CF_3).
4. **Hybridization**:
   - **sp^2 vs. sp^3**: sp^2 hybridized carbons are more electronegative than sp^3 hybridized carbons, making the conjugate base more stable.
   - **Example**: Phenol (C_6H_5OH) is more acidic than cyclohexanol ($C_6H_{11}OH$) because the phenoxide ion ($C_6H_5O^-$) is stabilized by resonance and the sp^2 hybridization of the aromatic ring.

7.3 Acid-Base Equilibria

Equilibrium Constants:

- **Ka**: The acid dissociation constant measures the extent to which an acid dissociates in water.

$HA \rightleftharpoons H^{+}+A^{-} K_a=[HA][H^{+}][A^{-}]$

- **Kb**: The base dissociation constant measures the extent to which a base dissociates in water.

$B+H_2O \rightleftharpoons BH^{+}+OH^{-} K_b=[B][BH^{+}][OH^{-}]$

Relationship Between Ka and Kb:

- **Water Autoionization**: The ion product of water (Kw) is given by:

$K_w=[H^{+}][OH^{-}]=1.0\times10^{-14}$ at $25^{\circ}C$

- **pKa and pKb**: The relationship between the pKa and pKb of conjugate acid-base pairs is:

$pK_a+pK_b=14$

7.4 Importance of Acids and Bases in Organic Chemistry

Catalysis:

- **Acid Catalysis**: Many organic reactions are catalyzed by acids. For example, the hydration of alkenes is catalyzed by acids.
- **Base Catalysis**: Many organic reactions are catalyzed by bases. For example, the hydrolysis of esters is catalyzed by bases.

Synthesis:

- **Nucleophilic Substitution**: Many nucleophilic substitution reactions involve the use of bases to deprotonate a nucleophile, making it more reactive.
- **Elimination Reactions**: Bases are often used to deprotonate a β-hydrogen, leading to the formation of a double bond.

Biological Systems:

- **Enzymes**: Many enzymes function as acid-base catalysts, facilitating reactions by donating or accepting protons.
- **pH Regulation**: The strength of acids and bases is crucial in maintaining the pH of biological systems, such as blood and cellular fluids.

7.5 Conclusion

Understanding the properties and behavior of organic acids and bases is essential for predicting and controlling the outcomes of chemical reactions. The pKa value is a key parameter in determining the strength of acids and the stability of their conjugate bases. By considering factors such as electronegativity, resonance stabilization, inductive effects, and hybridization, chemists can predict and manipulate the acidity and basicity of organic compounds. This knowledge is crucial in fields such as pharmaceuticals, biochemistry, and materials science

Chapter 8: Organic Reactions and Mechanisms

8.1 Types of Organic Reactions

- **Substitution Reactions**: Replacement of an atom or group by another.
- **Addition Reactions**: Addition of atoms or groups to unsaturated compounds.
- **Elimination Reactions**: Removal of atoms or groups to form unsaturated compounds.

8.2 Reaction Mechanisms

Mechanisms describe the step-by-step process of a reaction.

Example: Nucleophilic Substitution Reaction

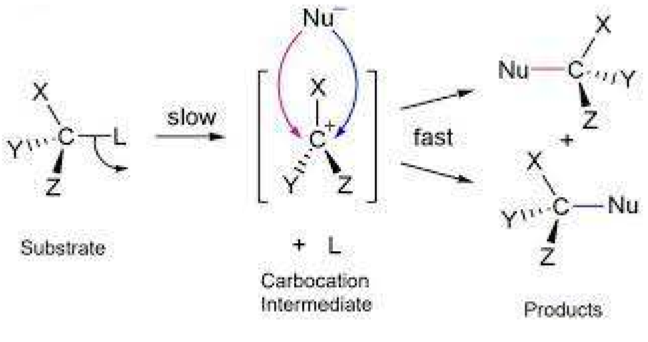
The reaction of bromoethane (C_2H_5Br) with hydroxide ion (OH^-) to form ethanol (C_2H_5OH) is a nucleophilic substitution reaction.

Chapter 8: Organic Reactions and Mechanisms

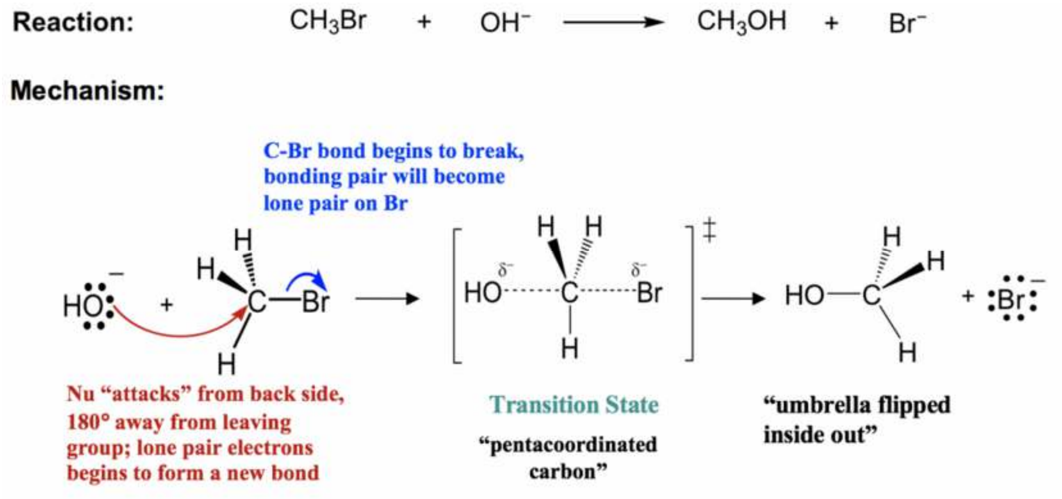
8.1 Types of Organic Reactions

Organic reactions can be classified into several types based on the nature of the reactants and the changes that occur during the reaction. Here are the main types of organic reactions:

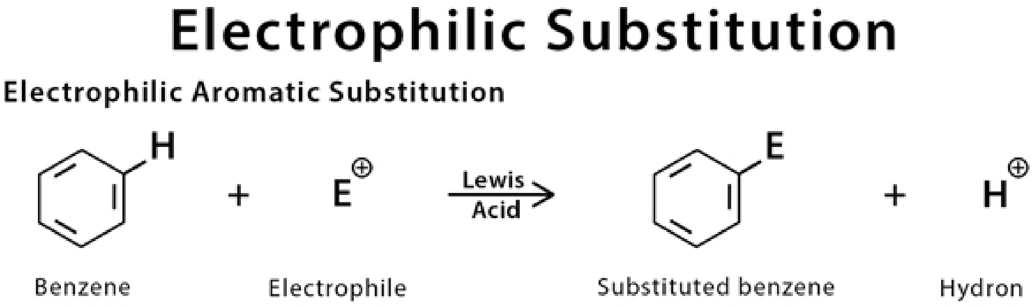
1. **Substitution Reactions**:
    - **Definition**: A substitution reaction involves the replacement of an atom or group in a molecule by another atom or group.
    - **Types**:
        - **Nucleophilic Substitution (NuS)**: A nucleophile (electron-rich species) replaces a leaving group (electron-poor species).
            - **Examples**:
                - **S_n1 Mechanism**: A two-step process where the leaving group departs first, forming a carbocation intermediate, which is then attacked by the nucleophile.
                - **Example**: Hydrolysis of tert-butyl bromide $(CH_3)_3CBr$ in water.



- **S_n2 Mechanism**: A one-step process where the nucleophile attacks the substrate while the leaving group departs simultaneously.
    - **Example**: Reaction of bromoethane (CH_3CH_2Br) with hydroxide ion (OH^-).

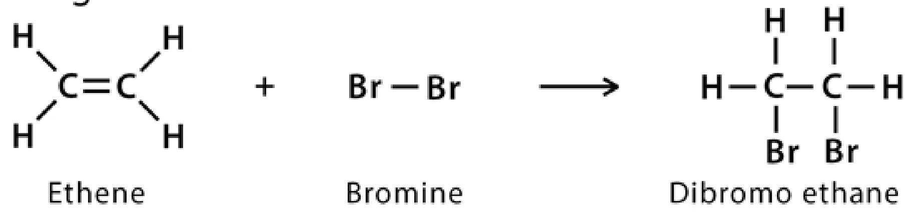


- **Electrophilic Substitution (ES)**: An electrophile (electron-poor species) replaces a hydrogen atom on an aromatic ring.
    - **Example**: Nitration of benzene (C_6H_6) with nitric acid (HNO_3) and sulfuric acid (H_2SO_4).

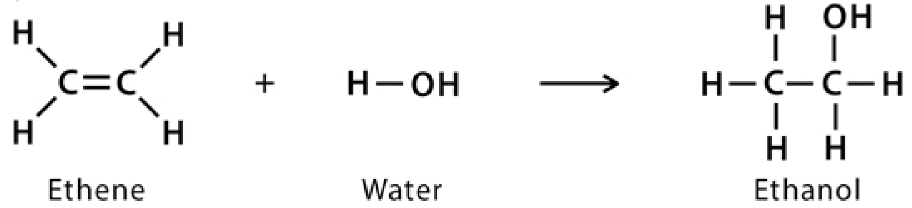


2. **Addition Reactions**:
    - **Definition**: An addition reaction involves the addition of atoms or groups to an unsaturated compound (e.g., alkenes, alkynes).
    - **Types**:
    - **Electrophilic Addition**: An electrophile adds to the double or triple bond, forming a new bond.
    - **Example**: Addition of hydrogen chloride (HCl) to ethene (C_2H_4).

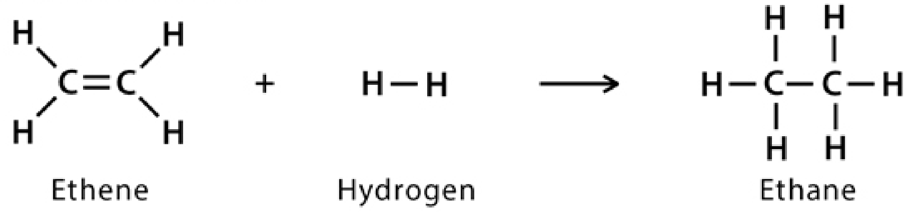
1. Halogenation



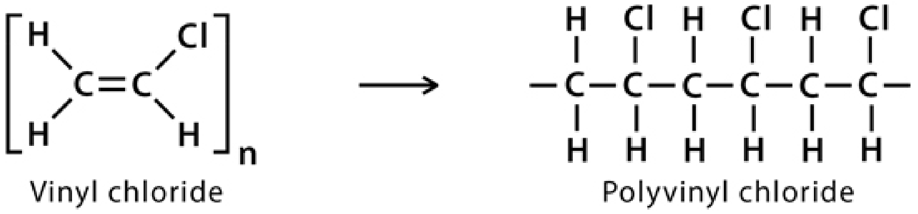
2. Hydration



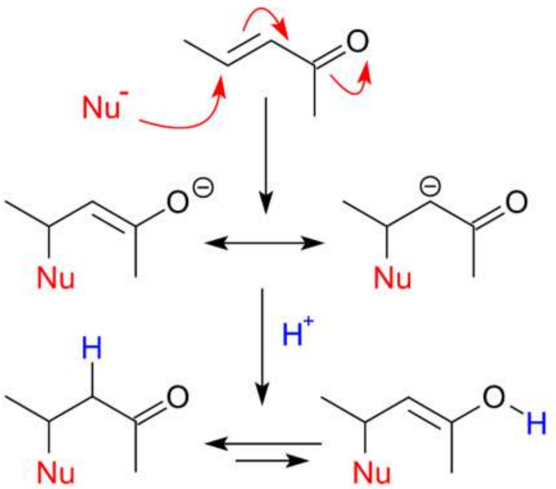
3. Hydrogenation



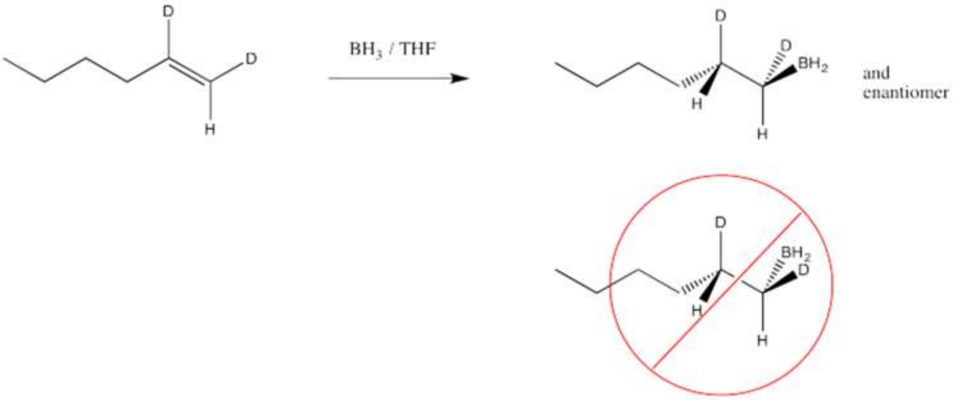
4. Polymerization



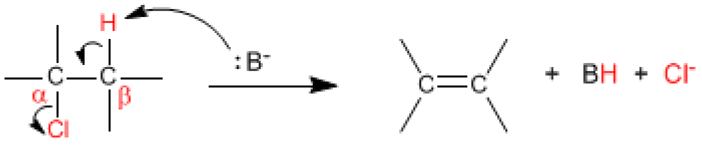
- **Nucleophilic Addition**: A nucleophile adds to the double or triple bond, forming a new bond.
- **Example**: Addition of cyanide ion (CN^-) to ethyne (C_2H_2).



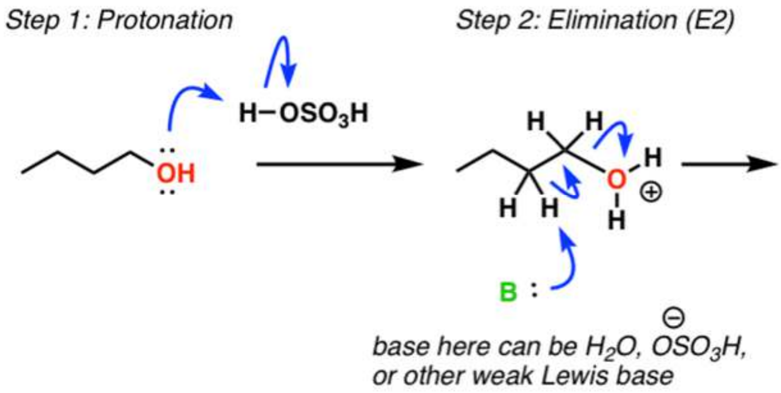
- **Concerted Addition**: Both reactants add simultaneously to the double or triple bond.
    - **Example**: Hydroboration of alkenes.



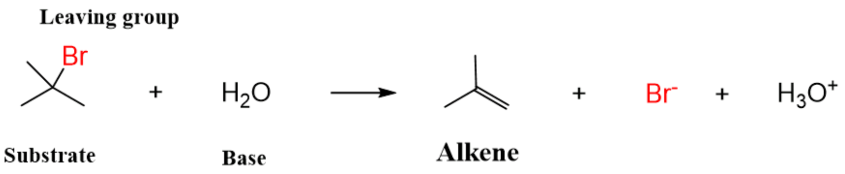
3. **Elimination Reactions**:
    - **Definition**: An elimination reaction involves the removal of atoms or groups from a molecule, forming an unsaturated compound (e.g., alkenes, alkynes).
    - **Types**:
    - **Beta-Elimination (E_2)**: A one-step process where a base abstracts a β-hydrogen, and the leaving group departs simultaneously, forming a double bond.
    - **Example**: Dehydrohalogenation of bromoethane (CH_3CH_2Br) with ethoxide ion ($CH_3CH_2O^-$).



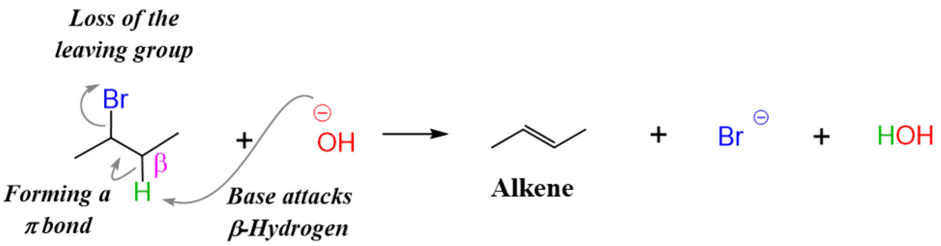
- **Unimolecular Elimination (E_1)**: A two-step process where the leaving group departs first, forming a carbocation intermediate, which then loses a proton to form a double bond.



  - **Example**: Dehydration of ethanol (CH_3CH_2OH) in the presence of an acid.



E1 - Elimination - Unimolecular



E2 Elimination - Binimolecular

8.2 Reaction Mechanisms

Reaction mechanisms describe the step-by-step process of a reaction, showing how reactants are converted into products. Understanding the mechanism is crucial for predicting the outcome of a reaction and controlling its conditions.

1. **Mechanism Elements**:
    - **Transition States**: High-energy intermediates that exist momentarily during the reaction.
    - **Intermediates**: Stable or unstable species that form during the reaction.
    - **Rate-Determining Step**: The slowest step in a multi-step reaction, which determines the overall rate of the reaction.
2. **Mechanistic Steps**:
    - **Bond Formation**: The formation of new bonds between atoms.
    - **Bond Breaking**: The breaking of existing bonds.
    - **Rearrangement**: The reorganization of atoms within a molecule.
3. **Examples of Mechanisms**:
    - **S_n2 Mechanism**:
        - **Step 1**: The nucleophile attacks the substrate from the opposite side of the leaving group.
        - **Step 2**: The leaving group departs simultaneously as the new bond forms.
        - **Example**: Reaction of bromoethane (CH_3CH_2Br) with hydroxide ion (OH^-).

          $CH_3CH_2Br+OH^- \rightarrow CH_3CH_2OH+Br^-$

    - **E_2 Mechanism**:
        - **Step 1**: The base abstracts a β-hydrogen.
        - **Step 2**: The leaving group departs simultaneously, forming a double bond.
        - **Example**: Dehydrohalogenation of bromoethane (CH_3CH_2Br) with ethoxide ion ($CH_3CH_2O^-$).

          CH3CH2Br+CH3CH2O−→CH2=CH2+CH3CH2OH+Br−

    - **Electrophilic Addition Mechanism**:
        - **Step 1**: The electrophile attacks the double bond, forming a carbocation intermediate.
        - **Step 2**: The nucleophile attacks the carbocation, forming the final product.
        - **Example**: Addition of hydrogen chloride (HCl) to ethene (C_2H_4).

          $C_2H_4+HCl \rightarrow CH_3CH_2Cl$

8.3 Importance of Reaction Mechanisms

Understanding reaction mechanisms is crucial for several reasons:

- **Predicting Reaction Outcomes**: Knowing the mechanism helps predict the products of a reaction and the conditions required to achieve the desired outcome.
- **Controlling Reaction Conditions**: By understanding the mechanism, chemists can control reaction conditions (e.g., temperature, solvent, concentration) to favor the desired pathway.
- **Designing Syntheses**: Mechanistic understanding is essential for designing efficient and selective synthetic routes to complex molecules.
- **Problem Solving**: Mechanistic insights help troubleshoot issues in reactions, such as low yields or unwanted side products.

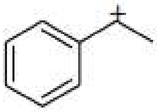
8.4 Conclusion

Organic reactions can be classified into substitution, addition, and elimination reactions, each with distinct mechanisms. Understanding these mechanisms is essential for predicting reaction outcomes, controlling reaction conditions, and designing efficient synthetic routes. By studying the step-by-step processes of reactions, chemists can gain valuable insights into the behavior of organic compounds and develop strategies for creating new molecules with desired properties

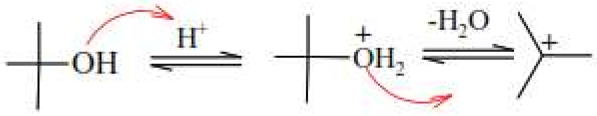
Exercise 1

1. Classify the following reactive species in descending order of stability:

$CH_3\text{-}\overset{+}{C}H\text{-}CH_2\text{-}CH_3$



2. The following two reactions can lead to carbocations

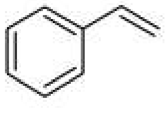
A) 

(planar carbocation structure)

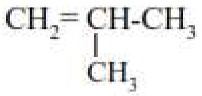
B) 

(planar carbocation structure)

Considering these two reactions, which carbocations can be formed from molecules A1, A2, and A3, and which one forms preferentially?

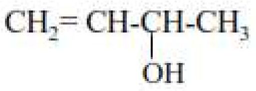


A1



$CH_2=\underset{\substack{|\\ CH_3}}{CH}-CH_3$

A2

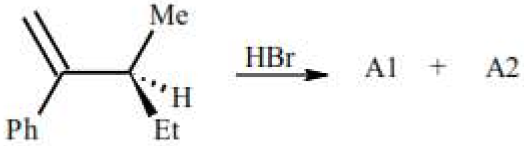


$CH_2=CH-\underset{\substack{|\\ OH}}{CH}-CH_3$

A3

Exercise 2

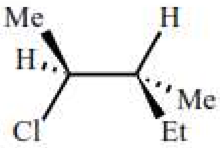
Consider the following reaction:



1. What type of reaction is this?
2. Detail the reaction mechanism, specifying the absolute configuration of A1 and A2.
3. What stereochemical relationship exists between A1 and A2?
4. Does the resulting mixture have optical activity?

Exercise 3

The treatment of compound A with hot sodium hydroxide leads to the formation of two products, one of which is majoritary.



A

1. Given that the rate is V = [A] [OH⁻], what type of reaction is this?
2. Detail the reaction mechanism and give the configuration of each product.

Exercise 4

Diethyl ether (A) is synthesized from ethanol in the presence of sulfuric acid.

1. Propose the synthesis of compound A according to an SN1 mechanism.
2. Propose the synthesis of compound A according to an SN2 mechanism.

Exercise 5

The 2-chloro-3-phenylbutane of absolute configuration (2S, 3S) is treated with sodium ethoxide (EtONa). A physicochemical analysis highlights two products with the molecular formulas $C_{10}H_{12}$ (compound A1) and $C_{12}H_{18}O$ (compound A2). One of the two products is optically active, and the other gives acetaldehyde and acetophenone upon ozonolysis in a reducing medium. Given that the reaction rate is of order 2.

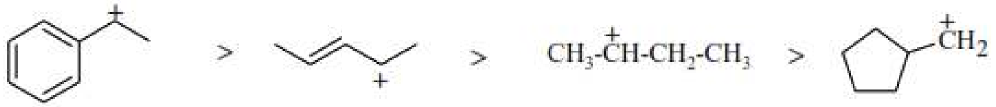
a) Detail the reaction schemes.

b) Specify the stereochemistry of compounds A1 and A2.

Solutions

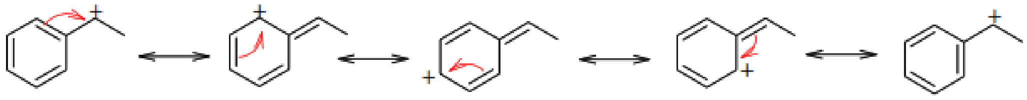
Exercise 1

1. Classification:



Secondary carbocation Primary carbocation

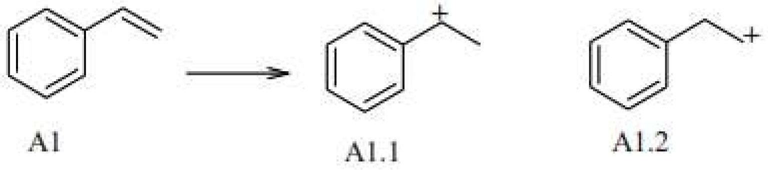
Two resonance forms



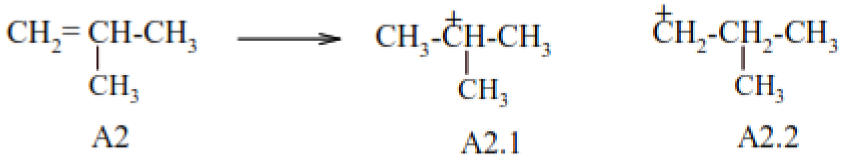
Five resonance forms

2.

- Compound A1 can lead to two carbocations A1.1 and A1.2. Carbocation A1.1 is stabilized by resonance (conjugated carbocation); it is therefore more stable and forms preferentially.

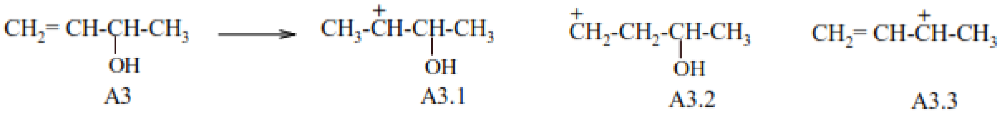


- Compound A2 can lead to two carbocations A2.1 and A2.2. Carbocation A2.1 is tertiary; it is therefore the most stable (it forms preferentially).



$$\underset{\text{A2}}{CH_2{=}\underset{\displaystyle CH_3}{\underset{|}{C}}H{-}CH_3} \longrightarrow \underset{\text{A2.1}}{CH_3{-}\underset{\displaystyle CH_3}{\underset{|}{\overset{+}{C}}}H{-}CH_3} \qquad \underset{\text{A2.2}}{\overset{+}{C}H_2{-}\underset{\displaystyle CH_3}{\underset{|}{C}}H_2{-}CH_3}$$

- Compound A3 can lead to three carbocations A3.1, A3.2, and A3.3. Carbocation A3.3 is stabilized by resonance, so it is the most stable (it forms preferentially).

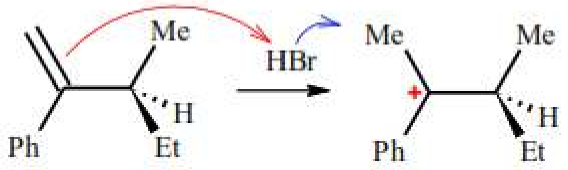


$$\underset{\text{A3}}{CH_2{=}CH{-}\underset{\displaystyle OH}{\underset{|}{C}}H{-}CH_3} \longrightarrow \underset{\text{A3.1}}{CH_3{-}\overset{+}{C}H{-}\underset{\displaystyle OH}{\underset{|}{C}}H{-}CH_3} \qquad \underset{\text{A3.2}}{\overset{+}{C}H_2{-}CH_2{-}\underset{\displaystyle OH}{\underset{|}{C}}H{-}CH_3} \qquad \underset{\text{A3.3}}{CH_2{=}CH{-}\overset{+}{C}H{-}CH_3}$$

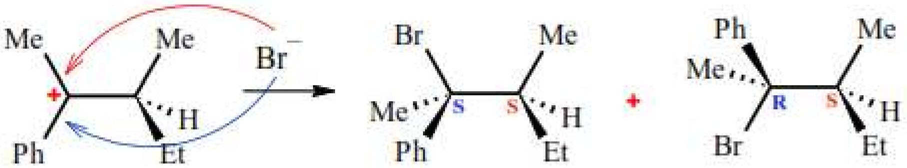
Exercise 2

1. It is an electrophilic addition reaction of H-Br on an alkene.
2. The reaction mechanism: the reaction proceeds in two steps

First step: In this step, the electrophile H^+ reacts with the π electrons of the double bond to form the most stable carbocation according to Markovnikov's rule.

-  Stable carbocation

Second step: In this step, the halide ion (Br^-) attacks the carbocation from both sides of the plane to form two molecules A1 and A2:

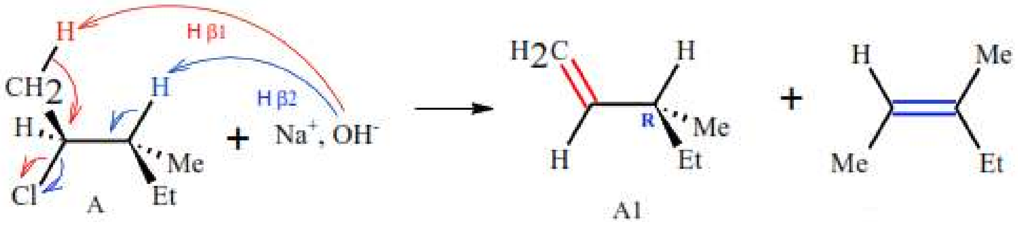


3. Molecules A1 and A2 are diastereomers.
4. The resulting mixture is chiral (since this mixture is not racemic).

Exercise 3

1. Since compound A is treated with hot sodium hydroxide, it is an elimination reaction, of type E2 because the reaction rate V = K [A] $[OH^-]$.

2. Since it is an E2 elimination reaction, it proceeds in a single step where the removal of the proton in the β position by the base, the departure of the nucleophile Cl^-, and the formation of the double bond occur simultaneously. It is also noted that the E2 reaction occurs when the proton in the β position and the nucleophile are in an antiperiplanar position. One alkene with Z or E configuration is obtained.



Remove H β1
Remove H β2

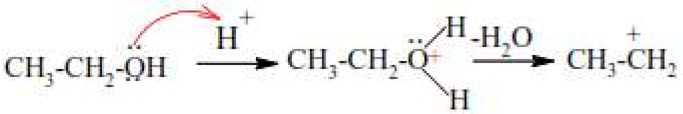
A2: Major alkene. Z configuration

The formation of the major product (A2) is justified by Zaitsev's rule (formation of the most substituted alkene).

Exercise 4

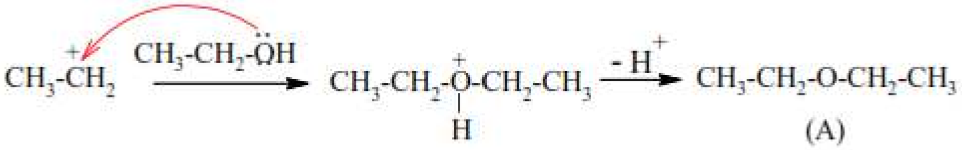
1. Synthesis of compound A according to an SN1 mechanism

The SN1 substitution reaction proceeds in two steps:
First step: In this step, a planar carbocation is formed.



$$CH_3\text{-}CH_2\text{-}\ddot{O}H \xrightarrow{H^+} CH_3\text{-}CH_2\text{-}\overset{+}{\ddot{O}}H_2 \xrightarrow{-H_2O} CH_3\text{-}\overset{+}{C}H_2$$

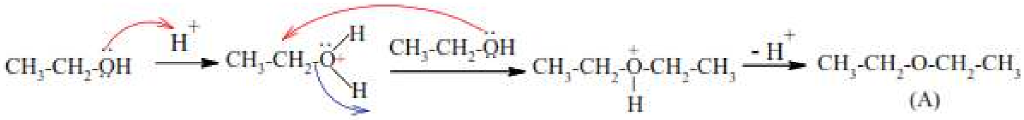
Second step: This step is characterized by the attack of the nucleophile ($CH_3\text{-}CH_2\text{-}OH$)



$$CH_3\text{-}\overset{+}{C}H_2 \xrightarrow{CH_3\text{-}CH_2\text{-}\ddot{O}H} CH_3\text{-}CH_2\text{-}\underset{H}{\overset{+}{O}}\text{-}CH_2\text{-}CH_3 \xrightarrow{-H^+} \underset{(A)}{CH_3\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_3}$$

2. Synthesis of compound A according to an SN2 mechanism

The SN2 substitution reaction proceeds in a single step during which the departure of the nucleophile and the attack of the nucleophile occur simultaneously.

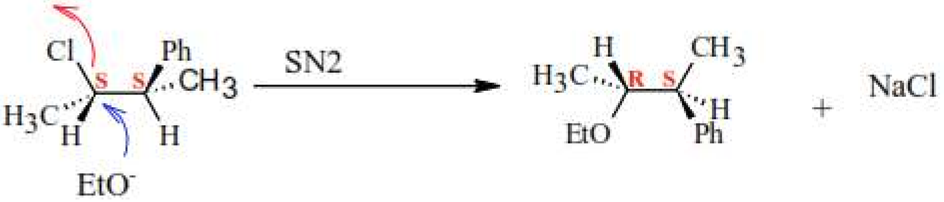


Exercise 5

Since the reaction rate is of order 2 (V= [2-chloro-3-phénylbutane]*[EtONa]), it is a bimolecular reaction, either SN2 or E2.

The formation of an optically active product is the result of an SN2 reaction. Meanwhile, the formation of another product that gives acetaldehyde and acetophenone upon ozonolysis in a reducing medium is the result of an E2 reaction.

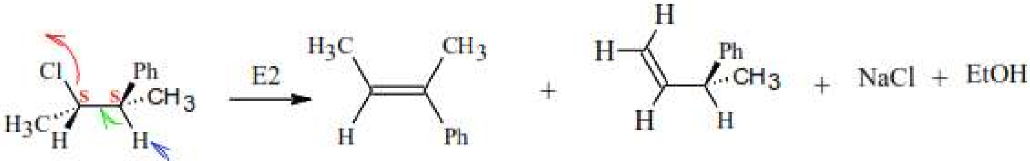
Reaction mechanism: SN2: $C_{12}H_{18}O$ (compound A2)



Walden inversion

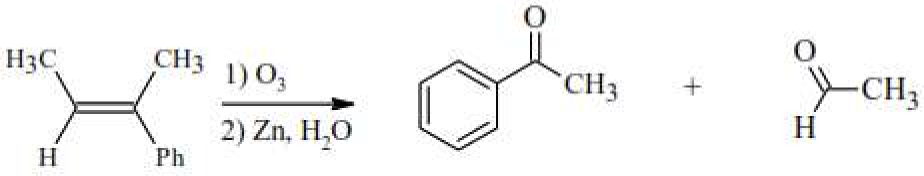
Optically active product

E2: $C_{10}H_{12}$ (compound A1)



Majoritary (most substituted), it respects Zaytsev's rule
Alkene of E configuration

Minoritary

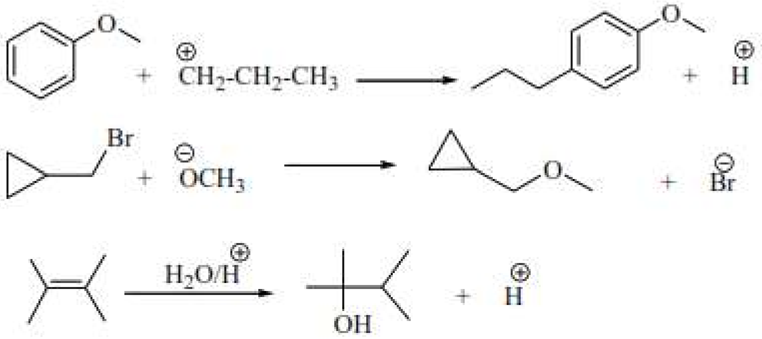


Acetophenone

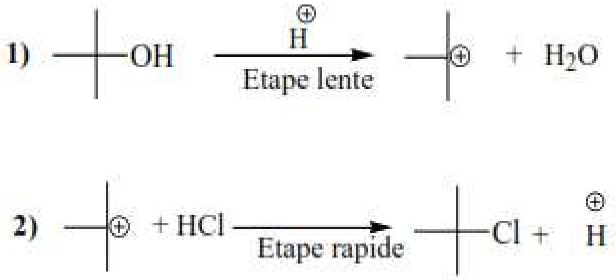
Acetaldehyde

Supplementary Exercise

Exercise 1: In the following series of reactions, indicate the substrate and the reagent. Specify the nature of the observed reaction.



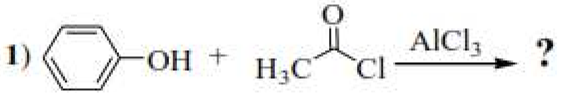
Exercise 2: Draw an energy diagram for the following reaction, which occurs in two steps:



Exercise 3: Among the following compounds, identify those that react via an SN1 mechanism. Justify.

a) CH_3-CH_2-CH_2-Cl
b) CH_2=CH-CH_2-Cl
c) C_6H_5-CH_2Cl
d) C_6H_5-CH_2-CH_2-Cl
e) $(CH_3)_3CCl$

Exercise 4: What are the products of the following reactions:



Exercise 5: Consider the following reactions:

1)

2)

Give the type and nature of the reaction that occurs, as well as the steps of the reaction mechanism. Is the reaction stereospecific? Justify.

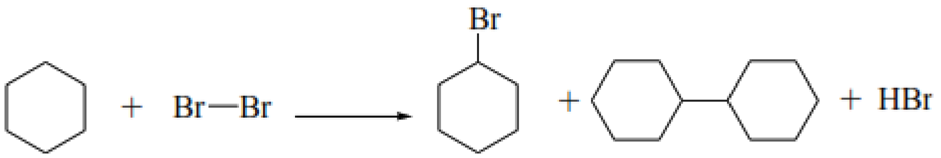
Exercise 6: (2R,3R) 3-phenylbutan-2-ol, treated with HCl, leads to 3-phenyl-2-chlorobutane. The mechanism is SN1, however, a specific rotation is observed for the reaction product. Propose an explanation, knowing that the substitution is complete.

Exercise 7: What is the product of the reaction of 3-bromo-3-methylhexane with OH- ions at high temperature? What would be the products of the reaction at any temperature?

Exercise 8:

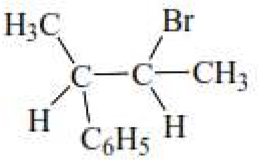
1. How can one achieve, in two steps (reactions), the transformation of 3-methylpentene to 3-methylpent-2-ene?
2. Detail the mechanism of the two reactions.

Exercise 9: Consider the following radical substitution reaction:



Detail the mechanism of the reaction.

Exercise 10: Consider compound A with the formula:



A

1. How many stereoisomers are there? Represent them in Fischer projection, specifying their respective configurations.
2. Represent the isomers (1S,2R) and (1R,2R) in Newman projection.
3. The optically active isomer of A with configuration (1S,2R) is treated with dilute sodium hydroxide (NaOH). The product obtained, B, is optically active.

Explain the type of reaction. Detail the mechanism of this reaction. Specify the configuration of B.

4. When the same isomer A is treated with concentrated sodium hydroxide, B and an inactive product C are obtained. What is the configuration of C? Detail the mechanism of this reaction.

Chapter 9: Alkanes and Cycloalkanes

9.1 Alkanes

Alkanes are saturated hydrocarbons with only single bonds.

9.2 Cycloalkanes

Cycloalkanes are alkanes with a ring structure.

Example: Cyclohexane (C_6H_{12})

Cyclohexane is a cycloalkane with six carbon atoms forming a ring.

Chapter 9: Alkanes and Cycloalkanes

9.1 Alkanes

Definition: Alkanes are saturated hydrocarbons that contain only single bonds between carbon atoms. They are the simplest class of organic compounds and form the basis for more complex organic molecules.
General Formula: The general formula for alkanes is C_nH_{2n+2}, where n is the number of carbon atoms.
Properties:

- **Physical State**: Alkanes with fewer than five carbon atoms are gases at room temperature, while those with more than five carbon atoms are liquids or solids.
- **Boiling and Melting Points**: These increase with increasing molecular weight due to stronger van der Waals forces.
- **Solubility**: Alkanes are non-polar and hydrophobic, meaning they are insoluble in water but soluble in non-polar solvents like hexane or benzene.
- **Chemical Reactivity**: Alkanes are generally unreactive due to the strong C-C and C-H single bonds. They typically undergo combustion and substitution reactions.

Examples:

- **Methane (CH_4)**: The simplest alkane, a major component of natural gas.
- **Ethane (C_2H_6)**: Used as a fuel and a raw material in the petrochemical industry.
- **Propane (C_3H_8)**: Commonly used as a fuel for heating and cooking.
- **Butane (C_4H_{10})**: Used in lighters and as a fuel for camping stoves.

Reactions:

- **Combustion**: Alkanes burn in the presence of oxygen to produce carbon dioxide and water.

$C_nH_{2n+2}+(23n+1)O_2 \rightarrow nCO_2 + (n+1)H_2O$

Example: Combustion of methane.

$CH_4+2O_2 \rightarrow CO_2+2H_2O$

- **Substitution Reactions**: Alkanes can undergo substitution reactions, particularly with halogens, in the presence of light or heat. **Example**: Chlorination of methane.

  $CH_4+Cl_2 \rightarrow CH_3Cl+HCl$

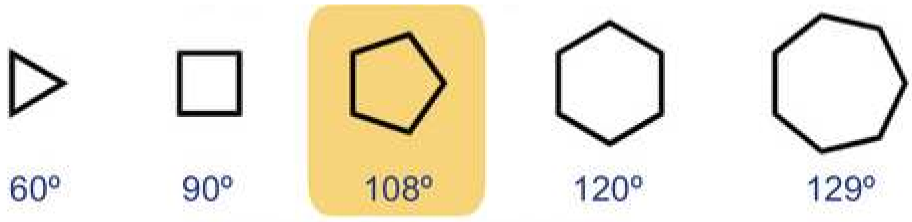
9.2 Cycloalkanes

Definition: Cycloalkanes are alkanes that form a closed ring structure. They are also saturated hydrocarbons but differ from alkanes in their ring structure, which can introduce strain and affect their properties.
General Formula: The general formula for cycloalkanes is CnH2n, where n is the number of carbon atoms in the ring.
Properties:

- **Ring Strain**: Small cycloalkanes (e.g., cyclopropane and cyclobutane) exhibit significant ring strain due to the deviation from ideal bond angles, making them more reactive than larger cycloalkanes.
- **Boiling and Melting Points**: Similar to alkanes, but generally higher due to the ring structure.
- **Solubility**: Like alkanes, cycloalkanes are non-polar and hydrophobic, insoluble in water but soluble in non-polar solvents.
- **Chemical Reactivity**: Cycloalkanes are generally more reactive than alkanes due to ring strain, especially in smaller rings.

Examples:

- **Cyclopropane (C_3H_6)**: A small, highly strained cycloalkane used as an anesthetic.
- **Cyclobutane (C_4H_8)**: Also strained, used in the synthesis of more complex molecules.
- **Cyclopentane (C_5H_{10})**: Less strained than cyclopropane and cyclobutane, used in the production of polystyrene.
- **Cyclohexane (C_6H_{12})**: A common solvent and starting material for the synthesis of nylon.



Internal C–C–C bond angles

Reactions:

- **Hydrogenation**: Cycloalkanes can be hydrogenated to form alkanes.

  Cycloalkane+H_2→Alkane

  Example: Hydrogenation of cyclohexane.

  $C_6H_{12}+6H_2 \rightarrow C_6H_{14}$

- **Halogenation**: Cycloalkanes can undergo halogenation, similar to alkanes, but the presence of ring strain can affect the reactivity. **Example**: Chlorination of cyclohexane.

  $C_6H_{12}+Cl_2 \rightarrow C_6H_{11}Cl+HCl$

- **Rearrangement Reactions**: Smaller cycloalkanes can undergo rearrangement reactions to relieve ring strain. **Example**: Cyclopropane can rearrange to form propene under certain conditions.

9.3 Importance of Alkanes and Cycloalkanes

Energy Sources:

- **Fuels**: Many alkanes, such as methane, propane, and butane, are used as fuels due to their high energy content and clean combustion.

Chemical Industry:

- **Raw Materials**: Alkanes and cycloalkanes are used as raw materials for the synthesis of more complex organic compounds, including polymers, pharmaceuticals, and solvents.

Biological Systems:

- **Lipids**: Cycloalkanes are components of many biological molecules, such as cholesterol and other steroids.

9.4 Conclusion

Alkanes and cycloalkanes are fundamental classes of organic compounds with diverse applications in energy, chemical synthesis, and biological systems. Understanding their properties and reactions is crucial for predicting their behavior and utilizing them effectively in various fields. The simplicity of alkanes and the unique properties of cycloalkanes due to ring strain make them essential components in the study and application of organic chemistry.

Chapter 10: Alkenes and Alkynes

10.1 Alkenes

Alkenes are hydrocarbons with at least one carbon-carbon double bond.

10.2 Alkynes

Alkynes have at least one carbon-carbon triple bond.

Example: Ethene (C_2H_4) and Ethyne (C_2H_2)

Ethene is an alkene with a double bond, while ethyne is an alkyne with a triple bond.

Chapter 10: Alkenes and Alkynes

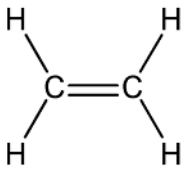
10.1 Alkenes

Definition: Alkenes are hydrocarbons that contain at least one carbon-carbon double bond (C=C). These double bonds make alkenes more reactive than alkanes due to the presence of a pi bond, which is more accessible to electrophiles and nucleophiles.
General Formula: The general formula for alkenes is C_nH_{2n}, where n is the number of carbon atoms.
Properties:

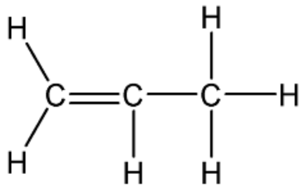
- **Physical State**: Alkenes with fewer than five carbon atoms are gases at room temperature, while those with more than five carbon atoms are liquids or solids.
- **Boiling and Melting Points**: These increase with increasing molecular weight due to stronger van der Waals forces.
- **Solubility**: Alkenes are non-polar and hydrophobic, meaning they are insoluble in water but soluble in non-polar solvents like hexane or benzene.
- **Chemical Reactivity**: Alkenes are more reactive than alkanes due to the presence of the double bond. They undergo addition reactions, where atoms or groups are added across the double bond.

Examples:

- **Ethene (C_2H_4)**: The simplest alkene, used in the production of polyethylene and other polymers.
- **Propene (C_3H_6)**: Used in the production of polypropylene and other chemicals.
- **Butene (C_4H_8)**: Used in the production of synthetic rubber and fuels.



Ethene



1-Propene

Reactions:

- **Addition Reactions**: Alkenes undergo addition reactions where atoms or groups are added across the double bond.
  - **Hydrogenation**: Addition of hydrogen to form alkanes.

    $C_nH_{2n}+H_2 \rightarrow C_nH_{2n+2}$

    Example: Hydrogenation of ethene.

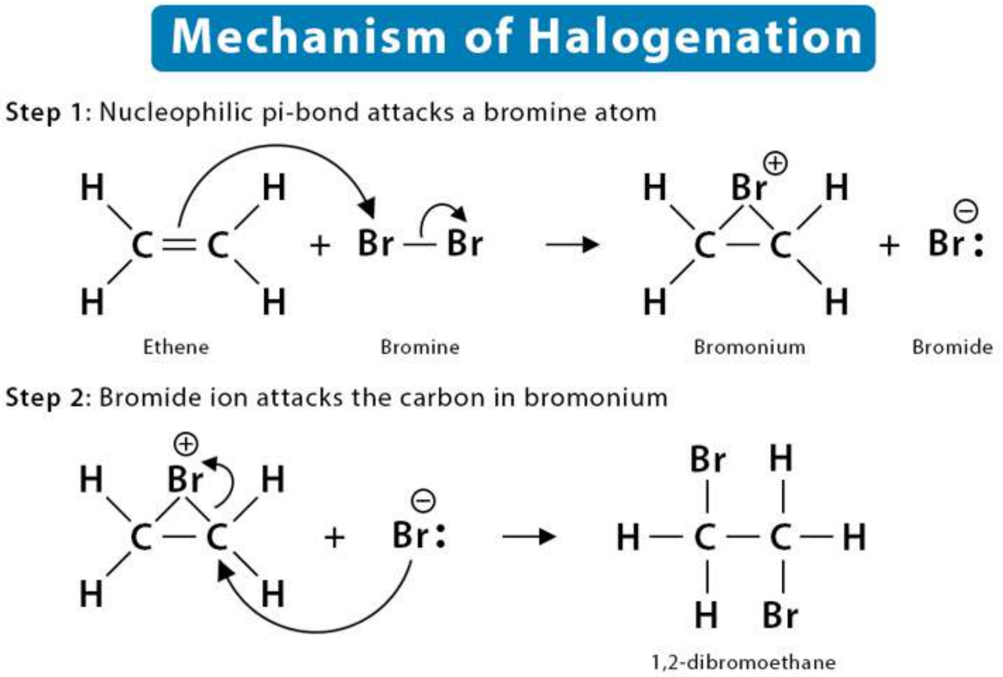
    $C_2H_4+H_2 \rightarrow C_2H_6$

  - **Halogenation**: Addition of halogens (e.g., bromine) to form dihalides.

    $C_nH_{2n}+X_2 \rightarrow C_nH_{2n}X_2$

    Example: Bromination of ethene.

    $C_2H_4+Br_2 \rightarrow C_2H_4Br_2$

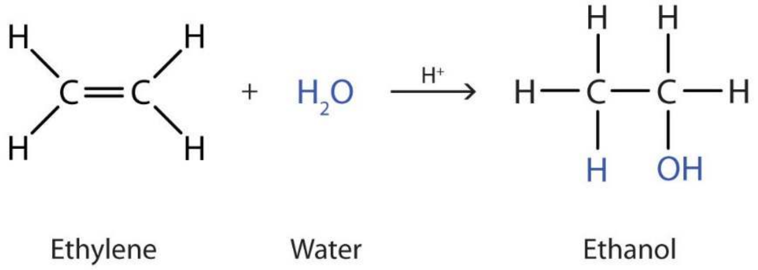


- **Hydration**: Addition of water to form alcohols.

  $C_nH_{2n}+H_2O \rightarrow C_nH_{2n+1}OH$

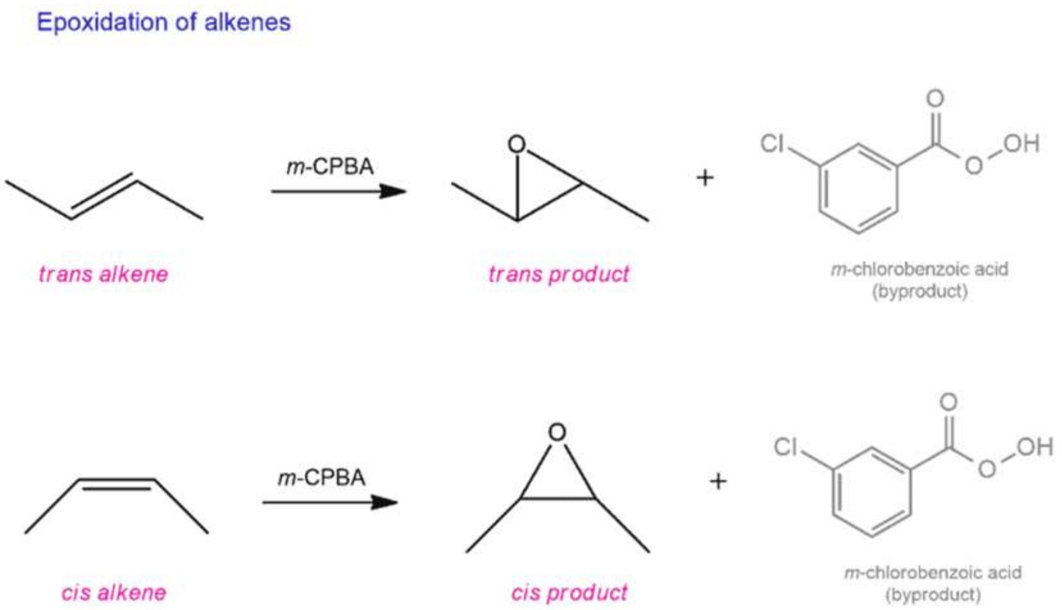
  Example: Hydration of ethene.

  $C_2H_4+H_2O \rightarrow C_2H_5OH$



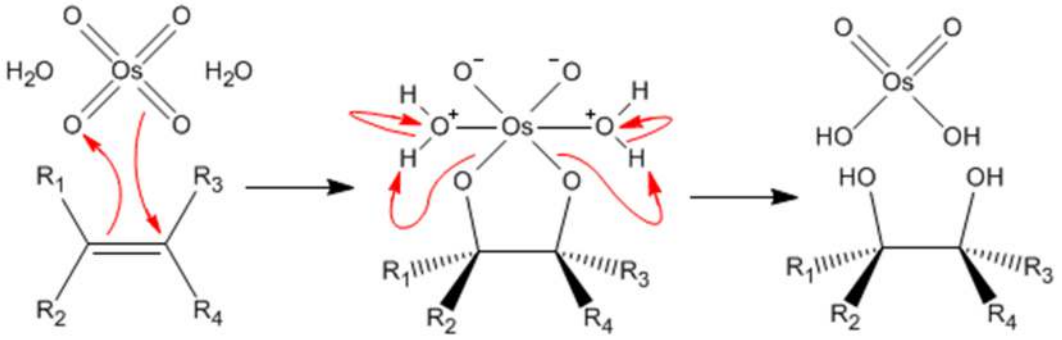
- **Oxidation Reactions**: Alkenes can be oxidized to form epoxides, diols, or ketones.
  - **Epoxidation**: Oxidation to form epoxides using reagents like m-chloroperoxybenzoic acid (mCPBA).

    $C_nH_{2n}+mCPBA \rightarrow C_nH_{2n}O$



- **Dihydroxylation**: Oxidation to form diols using reagents like osmium tetroxide (OsO_4).

  $C_nH_{2n}+OsO_4 \rightarrow C_nH_{2n}+2O_2$



10.2 Alkynes

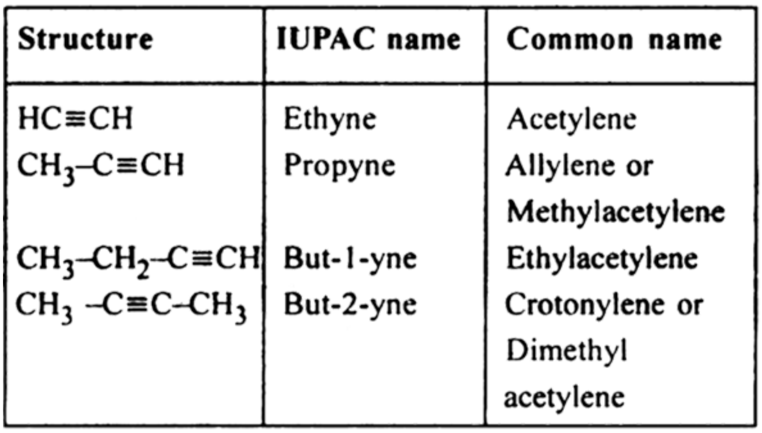
Definition: Alkynes are hydrocarbons that contain at least one carbon-carbon triple bond (C≡C). The triple bond consists of one sigma bond and two pi bonds, making alkynes highly reactive.
General Formula: The general formula for alkynes is CnH2n−2, where n is the number of carbon atoms.
Properties:

- **Physical State**: Alkynes with fewer than five carbon atoms are gases at room temperature, while those with more than five carbon atoms are liquids or solids.
- **Boiling and Melting Points**: These increase with increasing molecular weight due to stronger van der Waals forces.

- **Solubility**: Alkynes are non-polar and hydrophobic, meaning they are insoluble in water but soluble in non-polar solvents like hexane or benzene.
- **Chemical Reactivity**: Alkynes are more reactive than alkenes due to the presence of the triple bond. They undergo addition reactions, where atoms or groups are added across the triple bond.

Examples:

- **Ethyne (C_2H_2)**: The simplest alkyne, also known as acetylene, used in welding and cutting metals.
- **Propyne (C_3H_4)**: Used in the synthesis of various chemicals.
- **Butyne (C_4H_6)**: Used in the production of synthetic rubber and other chemicals.



Structure	IUPAC name	Common name
$HC\equiv CH$	Ethyne	Acetylene
$CH_3-C\equiv CH$	Propyne	Allylene or Methylacetylene
$CH_3-CH_2-C\equiv CH$	But-1-yne	Ethylacetylene
$CH_3-C\equiv C-CH_3$	But-2-yne	Crotonylene or Dimethyl acetylene

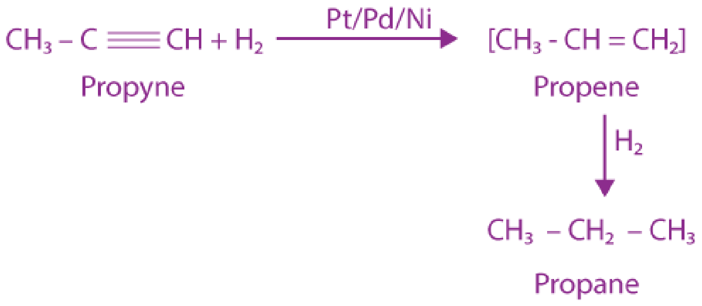
Reactions:

- **Addition Reactions**: Alkynes undergo addition reactions where atoms or groups are added across the triple bond.
    - **Hydrogenation**: Addition of hydrogen to form alkanes.

      $C_nH_{2n-2}+2H_2 \rightarrow C_nH_{2n+2}$

      Example: Hydrogenation of ethyne.

      $C_2H2+2H_2 \rightarrow C_2H_6$

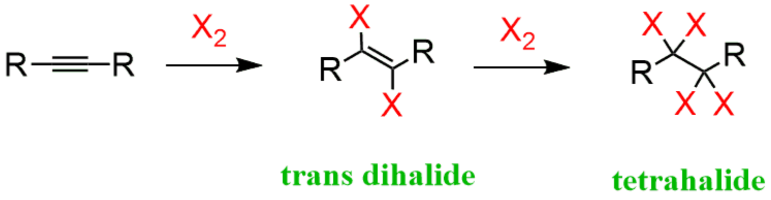


- **Halogenation**: Addition of halogens (e.g., bromine) to form tetrahalides.

  $C_nH_{2n-2}+2X_2 \rightarrow C_nH_{2n-2}X_4$

  Example: Bromination of ethyne.

  $C_2H_2+2Br_2 \rightarrow C_2H_2Br_4$

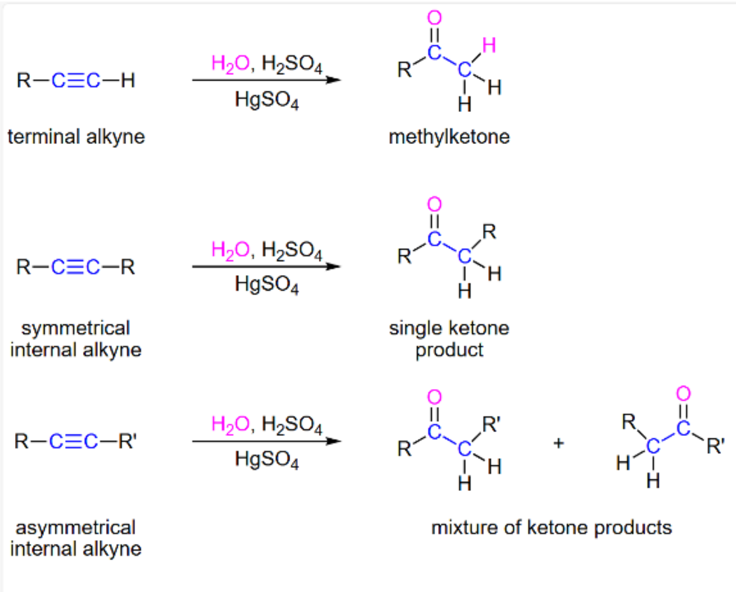


- **Hydration**: Addition of water to form aldehydes or ketones.

  $C_nH_{2n-2}+H_2O \rightarrow C_nH_{2n}O$

  Example: Hydration of ethyne.

  $C_2H_2+H_2O \rightarrow CH_3CHO$

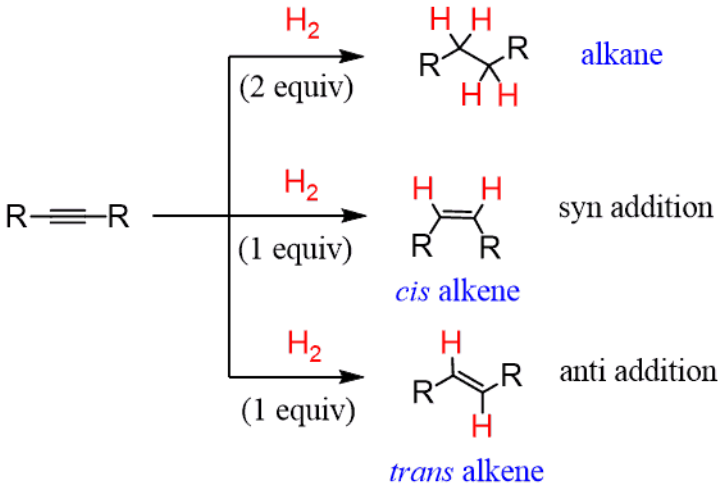


- **Reduction Reactions**: Alkynes can be reduced to form alkenes or alkanes.
    - **Partial Reduction**: Reduction to form alkenes using reagents like sodium borohydride ($NaBH_4$).

      $C_nH_{2n-2}+NaBH_4 \rightarrow C_nH_{2n}$

    - **Complete Reduction**: Reduction to form alkanes using reagents like hydrogen gas (H_2) and a metal catalyst (e.g., palladium on carbon, Pd/C).

      $CnH_{2n-2}+2H_2 \rightarrow CnH_{2n+2}$



10.3 Importance of Alkenes and Alkynes

Industrial Applications:

- **Polymers**: Alkenes are used as monomers in the production of polymers like polyethylene and polypropylene.
- **Synthetic Materials**: Alkynes are used in the synthesis of various chemicals, including acetylene for welding and cutting metals.

Chemical Synthesis:

- **Functional Group Transformations**: Alkenes and alkynes are versatile intermediates in organic synthesis, used to introduce various functional groups.
- **Cross-Coupling Reactions**: Alkynes are often used in cross-coupling reactions to form complex organic molecules.

Biological Systems:

- **Natural Products**: Alkenes and alkynes are components of many natural products, such as fatty acids and certain hormones.

10.4 Conclusion

Alkenes and alkynes are important classes of organic compounds with unique properties and reactivities due to the presence of double and triple bonds, respectively. Understanding their structures, properties, and reactions is crucial for their application in various fields, including industrial chemistry, materials science, and biological systems. The reactivity of alkenes and alkynes makes them valuable intermediates in organic synthesis, enabling the creation of a wide range of complex molecules.

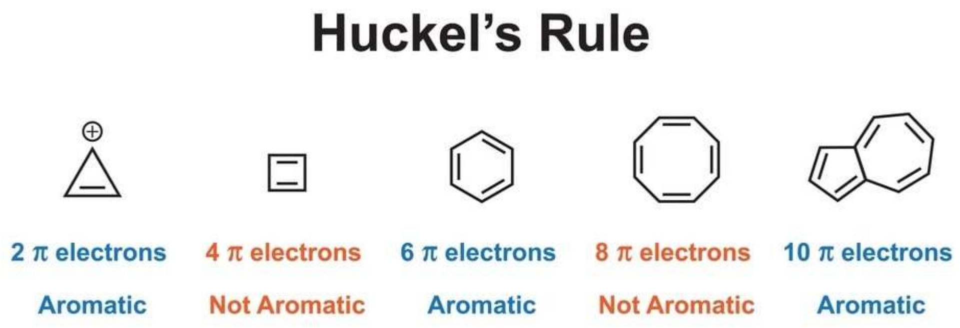
Chapter 11: Aromatic Compounds

11.1 Definition

Aromatic compounds have a ring structure with delocalized π-electrons, providing stability.

11.2 Aromaticity Rules

Aromatic compounds follow Hückel's rule, having (4n+2) π-electrons.



Example: Benzene (C_6H_6)

Benzene is a classic aromatic compound with six π-electrons.

Chapter 11: Aromatic Compounds

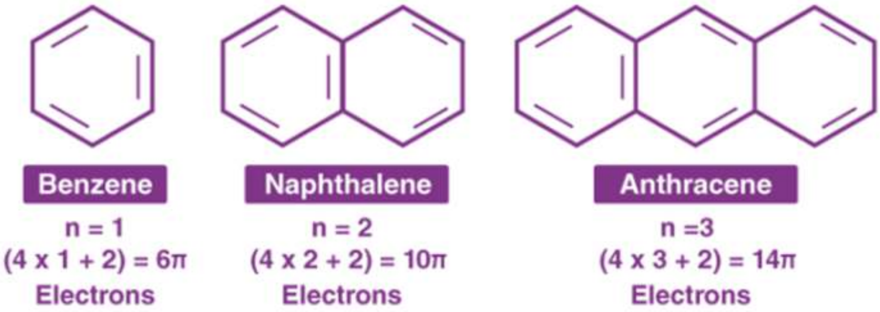
11.1 Definition

Definition: Aromatic compounds are a class of organic molecules characterized by a ring structure with delocalized π-electrons. This delocalization of electrons provides significant stability to these compounds, making them particularly resistant to reactions that would typically break double bonds in alkenes.
Key Features:

- **Ring Structure**: Aromatic compounds typically have a planar ring structure.
- **Delocalized π-Electrons**: The π-electrons are spread out over the entire ring, contributing to the stability of the molecule.
- **Resonance Structures**: Aromatic compounds often have multiple resonance structures, which further stabilize the molecule.

Examples:

- **Benzene (C_6H_6)**: The simplest and most well-known aromatic compound, with a six-membered ring and three double bonds.
- **Naphthalene ($C_{10}H_8$)**: A polycyclic aromatic hydrocarbon with two fused benzene rings.
- **Anthracene ($C_{14}H_{10}$)**: A polycyclic aromatic hydrocarbon with three fused benzene rings.



11.2 Aromaticity Rules

Hückel's Rule: Aromatic compounds follow Hückel's rule, which states that a molecule is aromatic if it has a continuous ring of overlapping p-orbitals containing $(4n+2)$ π-electrons, where n is an integer ($n = 0, 1, 2, 3, \ldots$).
Key Points of Hückel's Rule:

1. **Planarity**: The molecule must be planar to allow for the continuous overlap of p-orbitals.
2. **Conjugation**: The π-electrons must be delocalized over the entire ring.
3. **$(4n+2)$ π-Electrons**: The number of π-electrons must fit the formula $(4n+2)$, where n is an integer.

Examples:

- **Benzene (C_6H_6)**: Benzene has 6 π-electrons ($n = 1$ in Hückel's rule).

  $$4n+2=4(1)+2=6$$

  Benzene is aromatic and highly stable due to the delocalization of its π-electrons.

- **Cyclohexadiene (C_6H_8)**: Cyclohexadiene has 4 π-electrons ($n = 0.5$, which is not an integer).

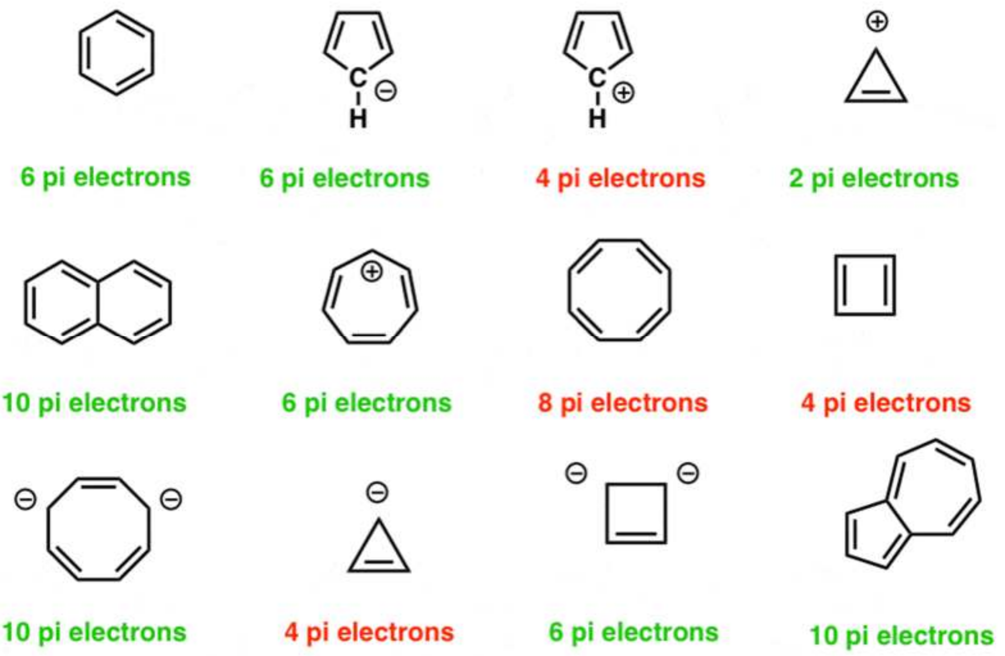
  $$4n+2=4(0.5)+2=4$$

  Cyclohexadiene is not aromatic and behaves like a typical diene.

- **Naphthalene ($C_{10}H_8$)**: Naphthalene has 10 π-electrons (n = 2 in Hückel's rule).

  $4n+2=4(2)+2=10$

  Naphthalene is aromatic and exhibits the stability associated with aromatic compounds.



Anti-Aromaticity: Compounds that have (4n) π-electrons are considered anti-aromatic and are typically less stable than aromatic compounds. For example, cyclobutadiene (C_4H_4) has 4 π-electrons (n = 1) and is anti-aromatic.
Non-Aromatic Compounds: Compounds that do not meet the criteria for aromaticity or anti-aromaticity are considered non-aromatic. For example, cyclohexane (C_6H_{12}) is a non-aromatic compound because it lacks a continuous ring of overlapping p-orbitals.

11.3 Properties of Aromatic Compounds

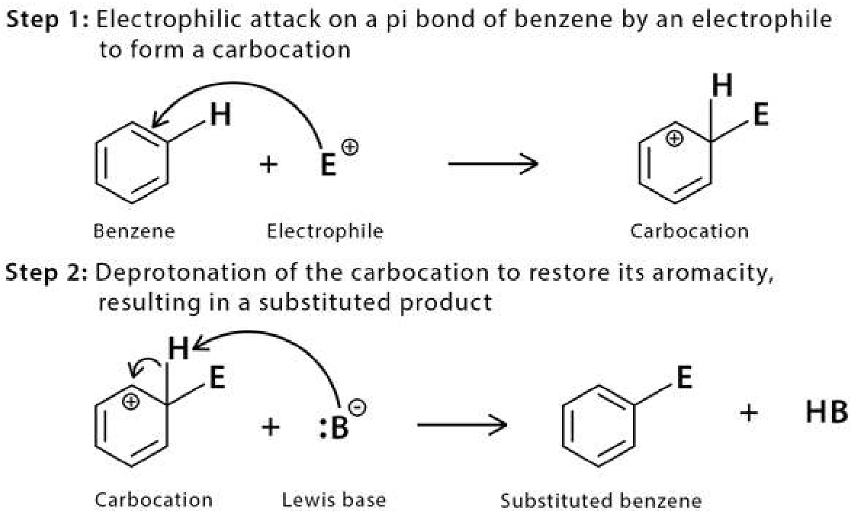
Stability:

- **Resonance Energy**: Aromatic compounds are more stable than their non-aromatic counterparts due to the delocalization of π-electrons, which is quantified as resonance energy.
- **Resistance to Reaction**: Aromatic compounds are less reactive than alkenes because the π-electrons are delocalized and more stable.

Reactions:

- **Electrophilic Aromatic Substitution**: Aromatic compounds typically undergo substitution reactions rather than addition reactions. Electrophiles can attack the aromatic ring, leading to the substitution of a hydrogen atom.

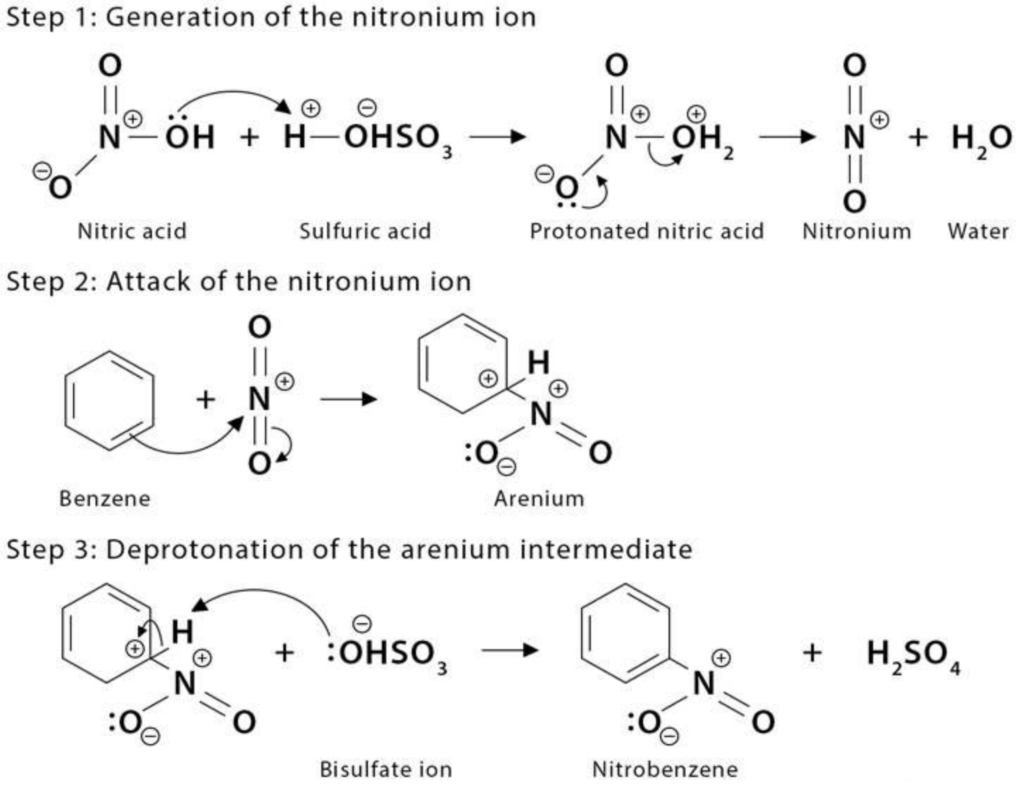
  $Ar\text{-}H + E^+ \rightarrow Ar\text{-}E + H^+$



Step 1: Electrophilic attack on a pi bond of benzene by an electrophile to form a carbocation

Step 2: Deprotonation of the carbocation to restore its aromacity, resulting in a substituted product

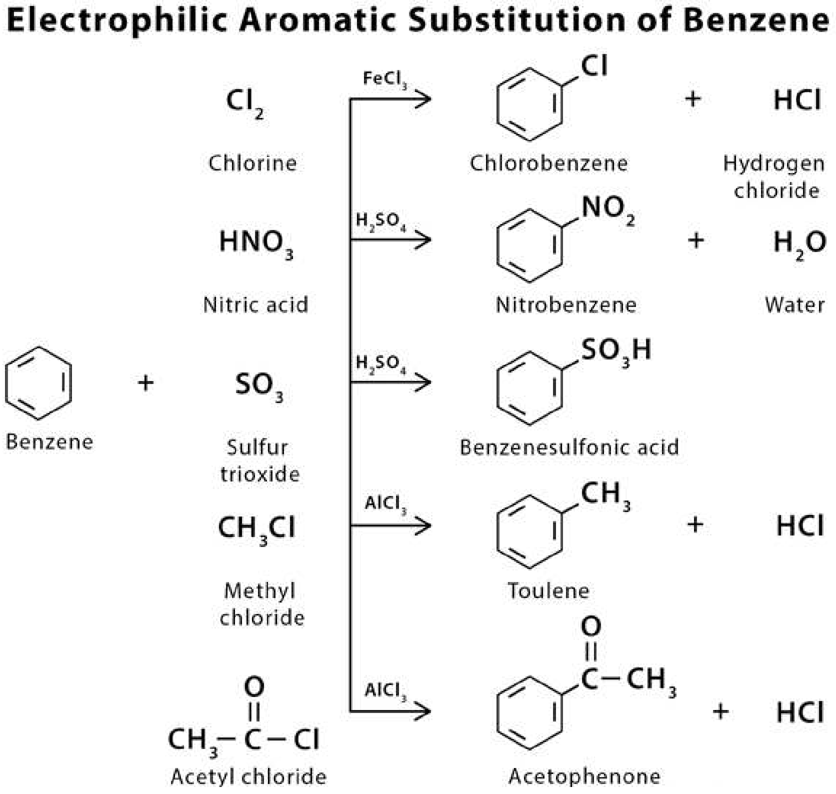
Example: Nitration of benzene. $C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$



Step 1: Generation of the nitronium ion

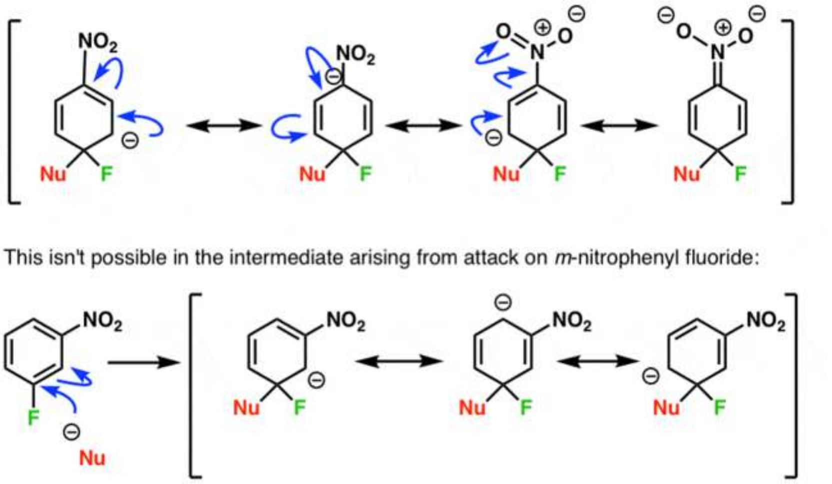
Step 2: Attack of the nitronium ion

Step 3: Deprotonation of the arenium intermediate


Electrophilic Aromatic Substitution of Benzene

- **Nucleophilic Aromatic Substitution**: Less common than electrophilic substitution, nucleophilic aromatic substitution involves the attack of a nucleophile on the aromatic ring.

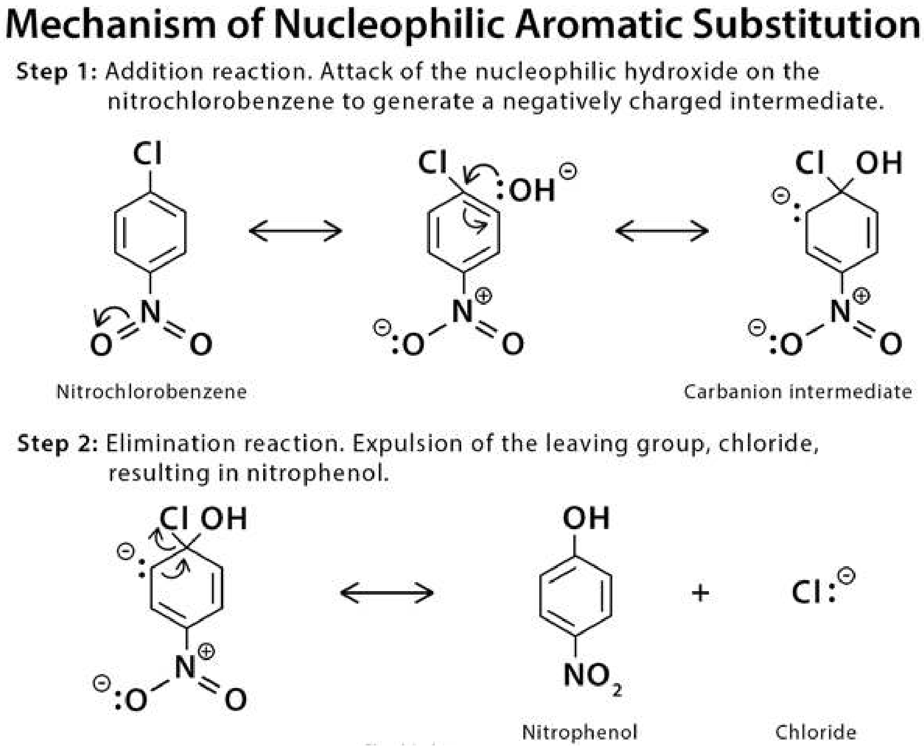
  $Ar\text{-}X+Nu^{-}\rightarrow Ar\text{-}Nu+X^{-}$



This isn't possible in the intermediate arising from attack on *m*-nitrophenyl fluoride:

Example: Substitution of a halogen by a hydroxide ion.

$$C_6H_5Cl + OH^- \rightarrow C_6H_5OH + Cl^-$$



11.4 Importance of Aromatic Compounds

Chemical Synthesis:

- **Starting Materials**: Aromatic compounds are widely used as starting materials in the synthesis of more complex organic molecules.
- **Functional Group Transformations**: The stability of aromatic compounds allows for selective functional group transformations without disrupting the aromatic system.

Biological Systems:

- **Natural Products**: Many natural products, such as hormones, vitamins, and alkaloids, contain aromatic rings.
- **Pharmaceuticals**: Aromatic compounds are common in pharmaceuticals, where they often contribute to the binding affinity and specificity of drugs.

Materials Science:

- **Polymers**: Aromatic compounds are used in the synthesis of polymers with unique properties, such as Kevlar and nylon.

- **Dyes and Pigments**: Aromatic compounds are used in the production of dyes and pigments due to their ability to absorb light in the visible spectrum.

11.5 Conclusion

Aromatic compounds are a unique and important class of organic molecules characterized by their ring structure and delocalized π-electrons. Understanding the principles of aromaticity, as described by Hückel's rule, is crucial for predicting the stability and reactivity of these compounds. Aromatic compounds play a vital role in various fields, including chemical synthesis, biological systems, and materials science, making them a fundamental topic in organic chemistry.

Chapter 12: Alcohols, Phenols, and Ethers

12.1 Alcohols

Alcohols contain an -OH group attached to a carbon atom.

12.2 Phenols

Phenols are aromatic alcohols with an -OH group attached to a benzene ring.

12.3 Ethers

Ethers have an -O- group linking two carbon atoms.

Example: Phenol (C_6H_5OH)

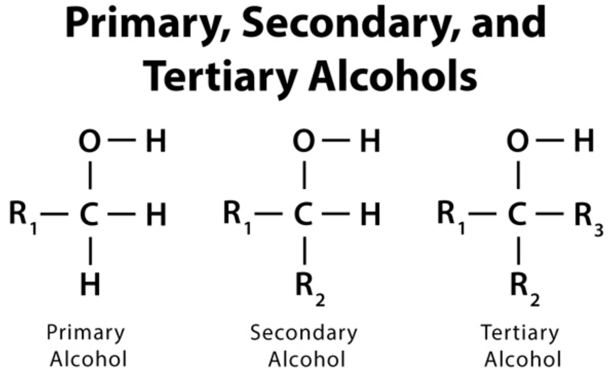
Phenol is an aromatic alcohol with an -OH group attached to a benzene ring.

Chapter 12: Alcohols, Phenols, and Ethers

12.1 Alcohols

Definition: Alcohols are organic compounds that contain an -OH (hydroxyl) group attached to a carbon atom. The presence of the -OH group makes alcohols polar and capable of forming hydrogen bonds.
General Formula: The general formula for alcohols is R-OH, where R represents an alkyl or aryl group.
Classification:

- **Primary Alcohols**: The -OH group is attached to a carbon atom that is bonded to at least one hydrogen atom.
  - **Example**: Ethanol (CH_3CH_2OH)
- **Secondary Alcohols**: The -OH group is attached to a carbon atom that is bonded to two other carbon atoms.
  - **Example**: Isopropanol ($CH_3CHOHCH_3$)
- **Tertiary Alcohols**: The -OH group is attached to a carbon atom that is bonded to three other carbon atoms.
  - **Example**: tert-Butanol ($(CH_3)_3COH$)



Properties:

- **Physical State**: Alcohols with low molecular weights are liquids at room temperature.
- **Boiling and Melting Points**: Higher than those of corresponding hydrocarbons due to hydrogen bonding.
- **Solubility**: Soluble in water due to hydrogen bonding with water molecules.
- **Chemical Reactivity**: Alcohols can undergo various reactions, including oxidation, esterification, and dehydration.

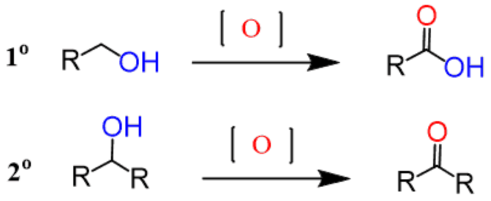
Reactions:

- **Oxidation**: Primary alcohols can be oxidized to aldehydes or carboxylic acids; secondary alcohols can be oxidized to ketones.
    - **Example**: Oxidation of ethanol to acetaldehyde.

$$CH_3CH_2OH \rightarrow CH_3CHO + H_2O$$

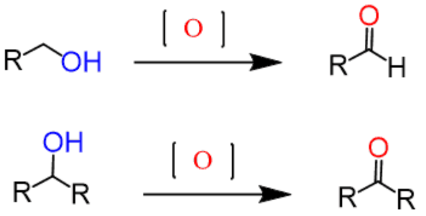
Oxidation of Alcohols using Strong and Mild Oxidizing Agents

Strong Oxidizing Agents oxidize **Primary Alcohols** to **Carboxylic Acids** and **Seconda** **Alcohols** to **Ketones**



$Na_2Cr_2O_7$/ H_2SO_4
H_2CrO_4
CrO_3/ H^+
$KMnO_4$/ ^-OH/ H^+
NaClO/ AcOH

Some oxidizing agents can **selectively oxidize primary alcohols to aldehyde:**



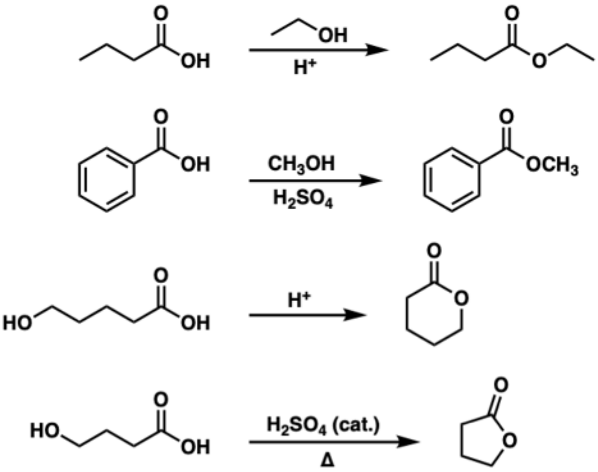
PCC (Pyridinium Chlorochromate)
PDC (Pyridinium Dichromate)
Swern (DMSO, $(COCl)_2$, Et_3N)
DMP (Dess-Martin)

Tertiary alcohols cannot be oxidized! (well, except for burning them to CO_2)

H is a must

- **Esterification**: Alcohols react with carboxylic acids to form esters.
    - **Example**: Esterification of ethanol with acetic acid.

$$CH_3CH_2OH + CH_3COOH \rightarrow CH_3COOCH_2CH_3 + H_2O$$

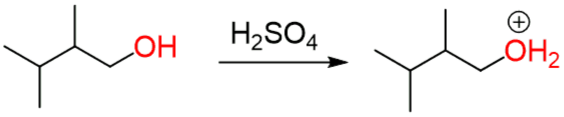


- **Dehydration**: Alcohols can lose water to form alkenes or ethers.
  - **Example**: Dehydration of ethanol to ethene.

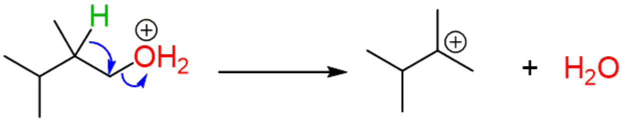
$CH_3CH_2OH \rightarrow C_2H_4 + H_2O$

Rearrangements in Dehydration of Primary Alcohols

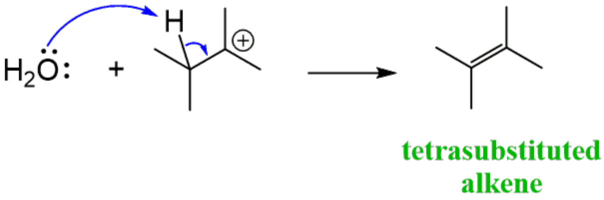
Step 1. *Protonation of the hydroxyl group*



Step 2. *1,2 shift of β-hydrogen forming a carbocation*



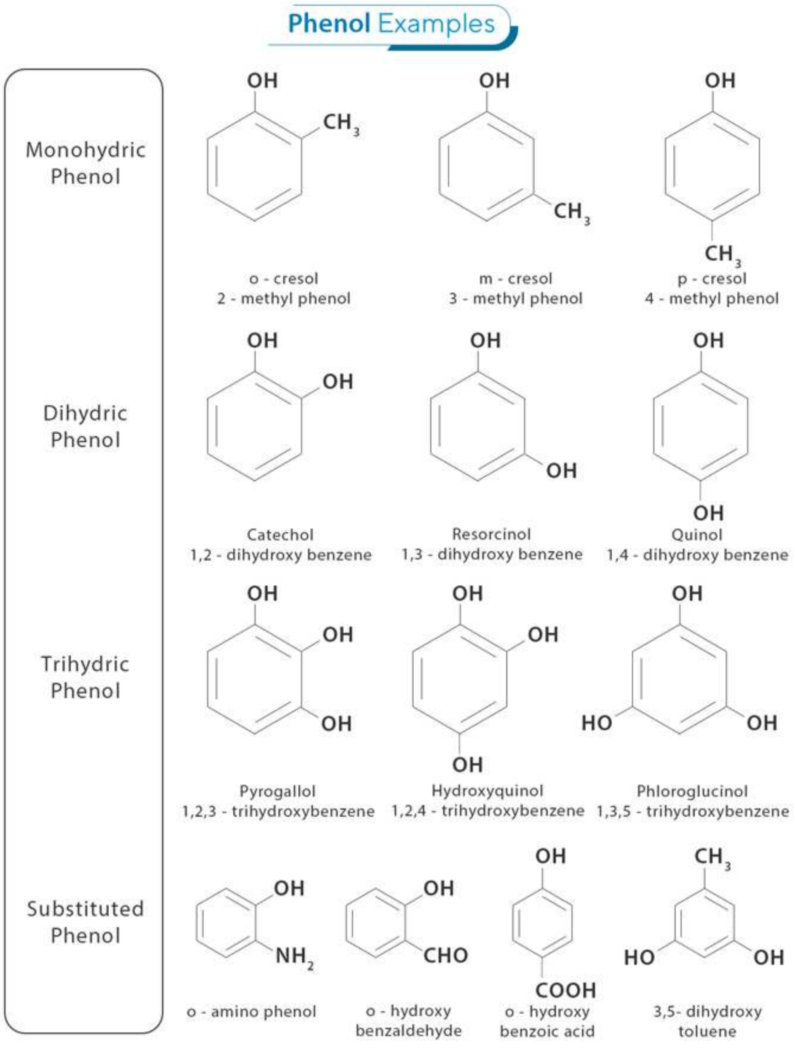
Step 3. *Removing β-hydrogen to form a π bond*



12.2 Phenols

Definition: Phenols are aromatic alcohols with an -OH group attached to a benzene ring. The aromatic ring influences the properties and reactivity of phenols.
General Formula: The general formula for phenols is Ar-OH, where Ar represents an aromatic ring.
Properties:

- **Physical State**: Phenols are typically liquids or solids at room temperature.
- **Boiling and Melting Points**: Higher than those of alcohols due to the aromatic ring.
- **Solubility**: Soluble in water due to hydrogen bonding.
- **Chemical Reactivity**: Phenols are more acidic than alcohols due to the resonance stabilization of the phenoxide ion.



Reactions:

- **Acid-Base Behavior**: Phenols are weak acids and can donate a proton to form phenoxide ions.
    - **Example**: Ionization of phenol.

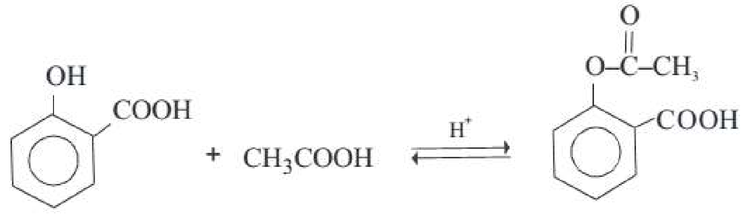
      $C_6H_5OH \rightleftharpoons C_6H_5O{-}+H_{+}$

- **Electrophilic Substitution**: Phenols can undergo electrophilic substitution reactions, such as nitration and bromination.
    - **Example**: Nitration of phenol.

      $C_6H_5OH+HNO_3 \rightarrow C_6H_4(OH)(NO2)+H2O$

- **Formation of Esters**: Phenols can react with carboxylic acids to form esters.
    - **Example**: Esterification of phenol with acetic acid.

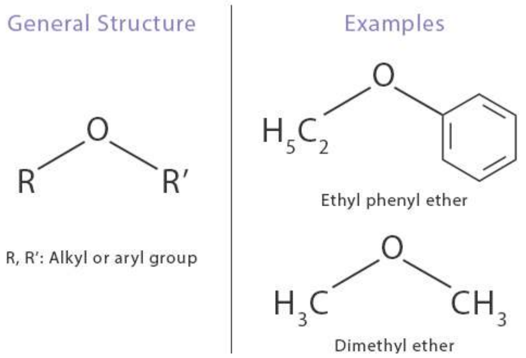
      $C_6H_5OH+CH_3COOH \rightarrow C_6H_5OCOCH_3+H_2O$



2-Hydroxybenzoic acid **Ethanoic acid** **Acetyl salicylic acid**

12.3 Ethers

Definition: Ethers are organic compounds that contain an -O- group linking two carbon atoms. The general formula for ethers is R-O-R’, where R and R’ can be the same or different alkyl or aryl groups.



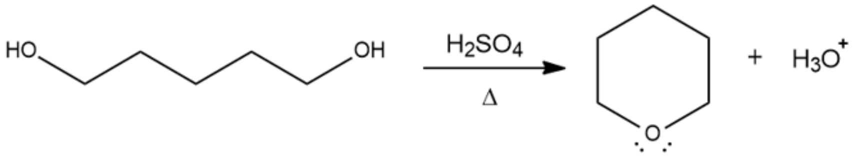
Properties:

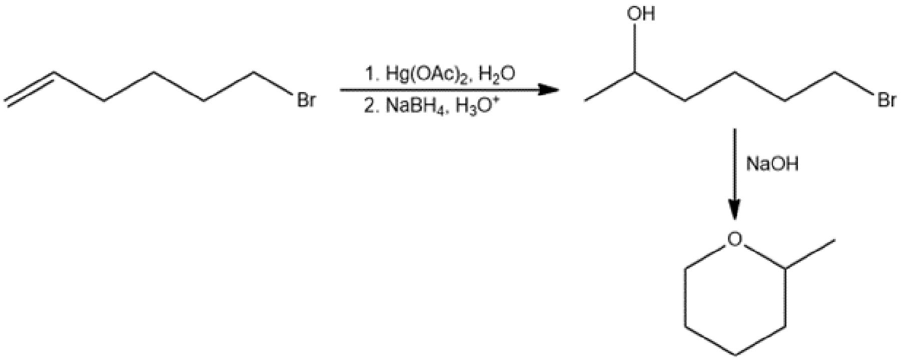
- **Physical State**: Ethers are typically liquids at room temperature.
- **Boiling and Melting Points**: Lower than those of alcohols due to the absence of hydrogen bonding.
- **Solubility**: Soluble in organic solvents but less soluble in water.
- **Chemical Reactivity**: Ethers are relatively unreactive but can undergo cleavage in the presence of strong acids or bases.

Reactions:

- **Cleavage**: Ethers can be cleaved by strong acids or bases to form alcohols.
  - **Example**: Cleavage of diethyl ether by hydroiodic acid.

$$CH_3CH_2OCH_2CH_3+2HI \rightarrow CH_3CH_2OH+CH_3CH_2I$$





- **Formation**: Ethers can be formed by the dehydration of alcohols or by the Williamson ether synthesis.
  - **Example**: Williamson ether synthesis.

$$CH_3CH_2ONa+CH_3I \rightarrow CH_3CH_2OCH_3+NaI$$

12.4 Importance of Alcohols, Phenols, and Ethers

Chemical Synthesis:

- **Starting Materials**: Alcohols, phenols, and ethers are commonly used as starting materials in organic synthesis.
- **Functional Group Transformations**: These compounds can undergo various reactions to introduce or transform functional groups.

Biological Systems:

- **Natural Products**: Many natural products, such as hormones, vitamins, and alkaloids, contain alcohol, phenol, or ether groups.
- **Pharmaceuticals**: These functional groups are often present in pharmaceuticals, contributing to their biological activity.

Industrial Applications:

- **Solvents**: Ethers, such as diethyl ether, are used as solvents in various industrial processes.
- **Plastics and Polymers**: Alcohols and phenols are used in the production of plastics and polymers.

12.5 Conclusion

Alcohols, phenols, and ethers are important classes of organic compounds with diverse properties and reactivities. Understanding their structures, properties, and reactions is crucial for their application in various fields, including chemical synthesis, biological systems, and industrial processes. The presence of the -OH and -O- groups in these compounds influences their reactivity and makes them valuable intermediates in organic chemistry

Chapter 13: Aldehydes and Ketones

13.1 Aldehydes

Aldehydes have a -CHO group.

13.2 Ketones

Ketones have a >C=O group.

Example: Acetaldehyde (CH_3CHO)

Acetaldehyde is an aldehyde with a -CHO group attached to a methyl group.

Chapter 13: Aldehydes and Ketones

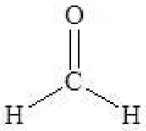
13.1 Aldehydes

Definition: Aldehydes are organic compounds that contain a -CHO group, where the carbonyl group (C=O) is bonded to at least one hydrogen atom and one carbon-containing group.
General Formula: The general formula for aldehydes is R-CHO, where R can be an alkyl or aryl group.
Properties:

- **Physical State**: Aldehydes with low molecular weights are gases at room temperature, while those with higher molecular weights are liquids or solids.
- **Boiling and Melting Points**: Higher than those of corresponding hydrocarbons due to the presence of polar carbonyl groups.
- **Solubility**: Soluble in water due to hydrogen bonding with water molecules.
- **Chemical Reactivity**: Aldehydes are more reactive than ketones due to the presence of a hydrogen atom adjacent to the carbonyl group, which can be oxidized.

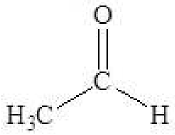
Examples:

- **Formaldehyde (HCHO)**: The simplest aldehyde, used in the production of resins and as a disinfectant.
- **Acetaldehyde (CH_3CHO)**: Used in the production of acetic acid and perfumes.
- **Benzaldehyde (C_6H_5CHO)**: An aromatic aldehyde used in the synthesis of dyes and perfumes.



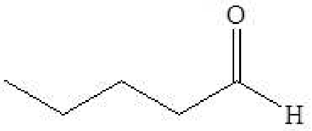
Methanal

(Formaldehyde)



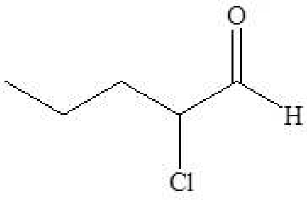
Ethanal

(Acetaldehyde)



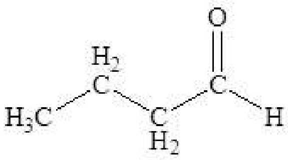
Pentanal

(Valeraldehyde)



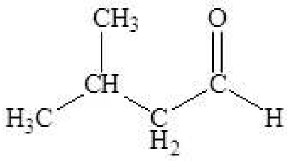
2-Chloropentanal

(a-Chlorovaleraldehyde)



Butanal

(Butyraldehyde)



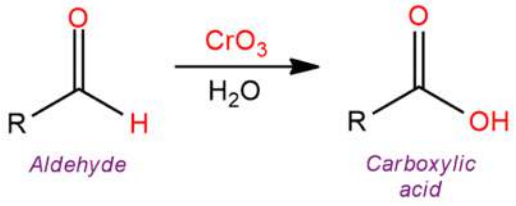
3-Methylbutanal

(isovaleraldehyde)

Reactions:

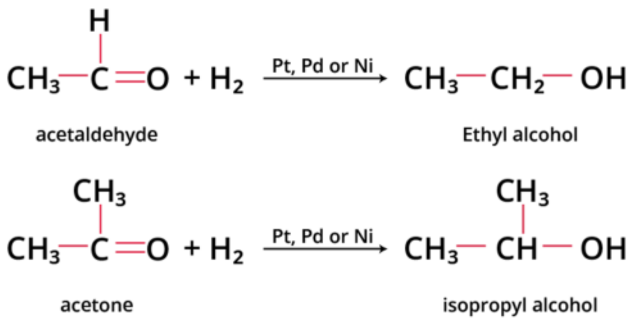
- **Oxidation**: Aldehydes can be oxidized to carboxylic acids.
    - **Example**: Oxidation of acetaldehyde to acetic acid.

$CH_3CHO+O_2 \rightarrow CH_3COOH$



- **Reduction**: Aldehydes can be reduced to alcohols.
    - **Example**: Reduction of acetaldehyde to ethanol.

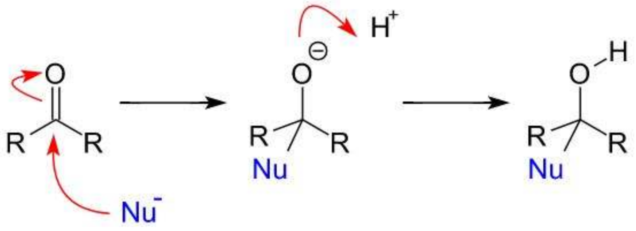
$CH_3CHO+H_2 \rightarrow CH_3CH_2OH$



$$CH_3-\overset{\overset{\displaystyle H}{|}}{C}=O + H_2 \xrightarrow{\text{Pt, Pd or Ni}} CH_3-CH_2-OH$$

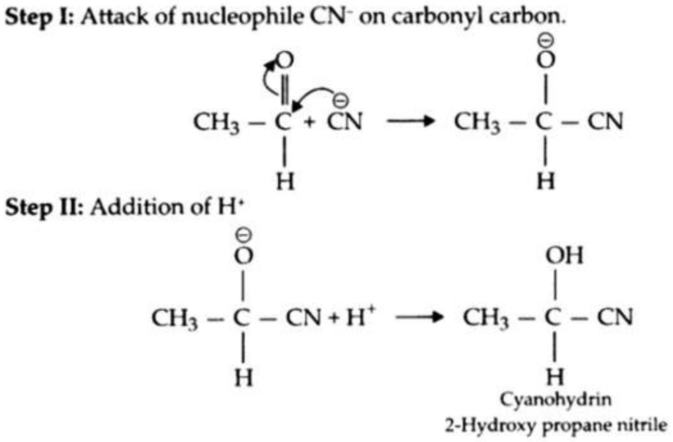
$$CH_3-\overset{\overset{\displaystyle CH_3}{|}}{C}=O + H_2 \xrightarrow{\text{Pt, Pd or Ni}} CH_3-\overset{\overset{\displaystyle CH_3}{|}}{CH}-OH$$

- **Nucleophilic Addition**: Aldehydes can undergo nucleophilic addition reactions, where nucleophiles attack the carbonyl carbon.



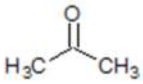
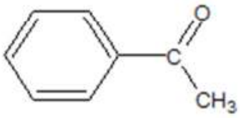
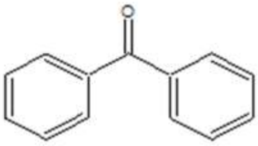
    - **Example**: Addition of hydrogen cyanide to acetaldehyde.

      $CH_3CHO+HCN \rightarrow CH_3CH(OH)CN$



13.2 Ketones

Definition: Ketones are organic compounds that contain a >C=O group, where the carbonyl group (C=O) is bonded to two carbon-containing groups.
General Formula: The general formula for ketones is R-CO-R', where R and R' can be the same or different alkyl or aryl groups.

Compound	Systematic	Common
	propane ↓ propanone	acetone or dimethyl ketone
	1-phenylethane ↓ 1-phenylethanone	acetophenone or methyl phenyl ketone
	benzophenone	diphenyl ketone

Properties:

- **Physical State**: Ketones with low molecular weights are liquids at room temperature.
- **Boiling and Melting Points**: Higher than those of corresponding hydrocarbons due to the presence of polar carbonyl groups.
- **Solubility**: Soluble in water due to hydrogen bonding with water molecules.
- **Chemical Reactivity**: Ketones are less reactive than aldehydes because they lack the hydrogen atom adjacent to the carbonyl group, which makes them less susceptible to oxidation.

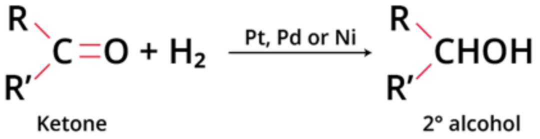
Examples:

- **Acetone (CH_3COCH_3)**: A common solvent used in nail polish remover and as a cleaning agent.
- **Butanone ($CH_3COCH_2CH_3$)**: Used as a solvent and in the production of plastics.
- **Cyclohexanone ($C_6H_{10}O$)**: Used in the production of nylon and other polymers.

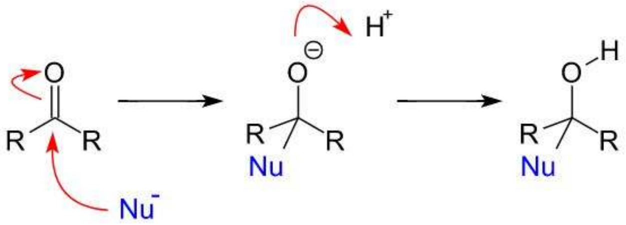
Reactions:

- **Reduction**: Ketones can be reduced to secondary alcohols.
  - **Example**: Reduction of acetone to isopropanol.

$CH_3COCH_3 + H_2 \rightarrow CH_3CHOHCH_3$

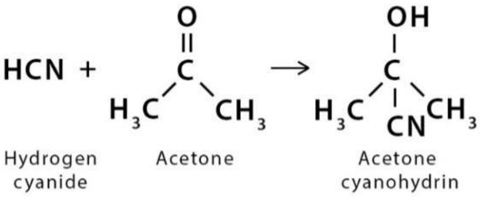


- **Nucleophilic Addition**: Ketones can undergo nucleophilic addition reactions, where nucleophiles attack the carbonyl carbon.



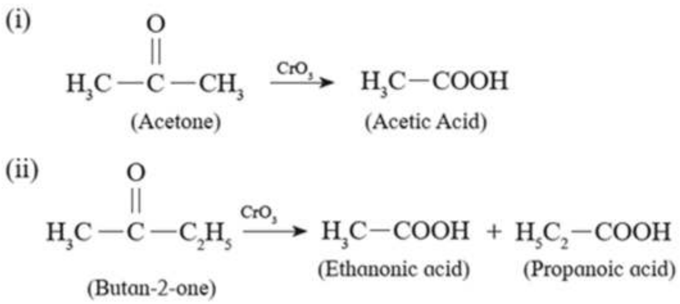
  - **Example**: Addition of hydrogen cyanide to acetone.

$CH_3COCH_3 + HCN \rightarrow CH_3COCH_2CN$



- **Oxidation**: Ketones are generally resistant to oxidation, but under extreme conditions, they can be oxidized to carboxylic acids.
- Reduction: Ketones : with example in english
  - **Example**: Oxidation of acetone to acetic acid.

$CH_3COCH_3 + 3O_2 \rightarrow 2CH_3COOH$



$(i)\; H_3C-\overset{\overset{O}{||}}{C}-CH_3 \xrightarrow{CrO_3} H_3C-COOH$

$(ii)\; H_3C-\overset{\overset{O}{||}}{C}-C_2H_5 \xrightarrow{CrO_3} H_3C-COOH + H_5C_2-COOH$

13.3 Importance of Aldehydes and Ketones

Chemical Synthesis:

- **Starting Materials**: Aldehydes and ketones are commonly used as starting materials in organic synthesis.
- **Functional Group Transformations**: These compounds can undergo various reactions to introduce or transform functional groups.

Biological Systems:

- **Natural Products**: Many natural products, such as hormones, vitamins, and alkaloids, contain aldehyde or ketone groups.
- **Metabolic Pathways**: Aldehydes and ketones are intermediates in various metabolic pathways.

Industrial Applications:

- **Solvents**: Ketones, such as acetone, are used as solvents in various industrial processes.
- **Plastics and Polymers**: Aldehydes and ketones are used in the production of plastics and polymers.

13.4 Conclusion

Aldehydes and ketones are important classes of organic compounds with diverse properties and reactivities. Understanding their structures, properties, and reactions is crucial for their application in various fields, including chemical synthesis, biological systems, and industrial processes. The presence of the -CHO and >C=O groups in these compounds influences their reactivity and makes them valuable intermediates in organic chemistry.

Chapter 14: Carboxylic Acids and Derivatives

14.1 Carboxylic Acids

Carboxylic acids have a -COOH group.

14.2 Derivatives

Derivatives include esters, anhydrides, and amides.

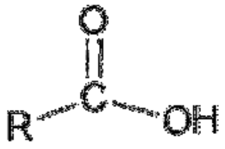
Example: Acetic Acid (CH_3COOH)

Acetic acid is a carboxylic acid with a -COOH group attached to a methyl group.

Chapter 14: Carboxylic Acids and Derivatives

14.1 Carboxylic Acids

Definition: Carboxylic acids are organic compounds that contain a -COOH group, where the carbonyl group (C=O) is bonded to a hydroxyl group (-OH).
General Formula: The general formula for carboxylic acids is R-COOH, where R can be an alkyl or aryl group.



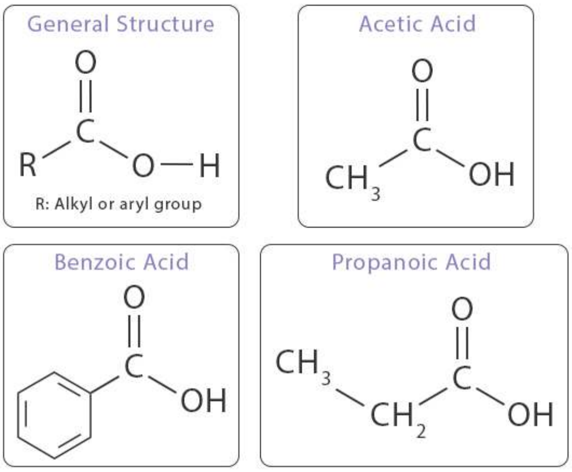
Carboxylic acid

Properties:

- **Physical State**: Carboxylic acids with low molecular weights are liquids at room temperature, while those with higher molecular weights are solids.
- **Boiling and Melting Points**: Higher than those of corresponding alcohols due to the presence of hydrogen bonding.
- **Solubility**: Soluble in water due to hydrogen bonding with water molecules.
- **Chemical Reactivity**: Carboxylic acids are acidic and can donate a proton (H^+) to form carboxylate ions.

Examples:

- **Formic Acid ($HCOOH$)**: The simplest carboxylic acid, found in ant venom.
- **Acetic Acid (CH_3COOH)**: A common carboxylic acid, used in vinegar and in the production of polymers.
- **Benzoic Acid (C_6H_5COOH)**: An aromatic carboxylic acid, used as a preservative and in the synthesis of dyes and perfumes.



Reactions:

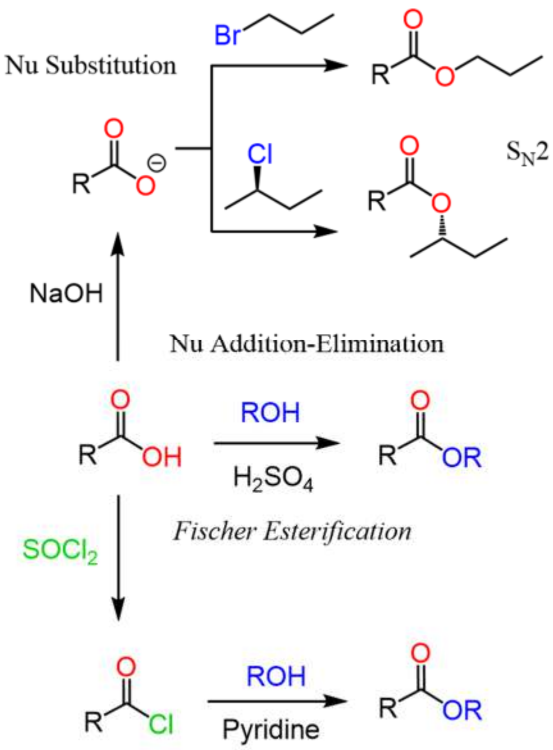
- **Acid-Base Behavior**: Carboxylic acids can donate a proton to form carboxylate ions.
    - **Example**: Ionization of acetic acid.

      $CH3COOH \rightleftharpoons CH3COO^{-}+H^{+}$

- **Esterification**: Carboxylic acids can react with alcohols to form esters.
    - **Example**: Esterification of acetic acid with ethanol.

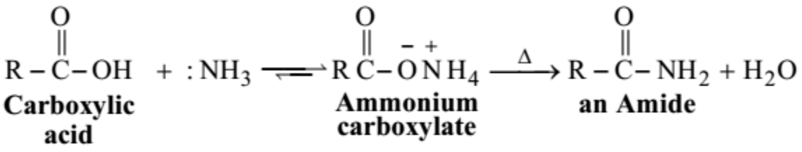
      $CH_3COOH+CH_3CH_2OH \rightarrow CH_3COOCH_2CH_3+H_2O$

Converting Carboxylic Acids to Esters



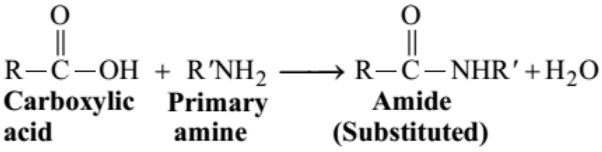
- **Amidation**: Carboxylic acids can react with amines to form amides.
    - **Example**: Amidation of acetic acid with ammonia.

$CH_3COOH+NH_3 \rightarrow CH_3CONH_2+H_2O$



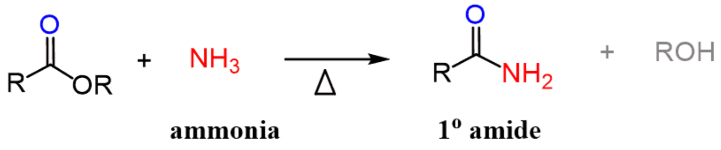
$$R-\overset{O}{\overset{\|}{C}}-OH + :NH_3 \rightleftharpoons R\overset{O}{\overset{\|}{C}}-\overset{-}{O}\overset{+}{N}H_4 \xrightarrow{\Delta} R-\overset{O}{\overset{\|}{C}}-NH_2 + H_2O$$

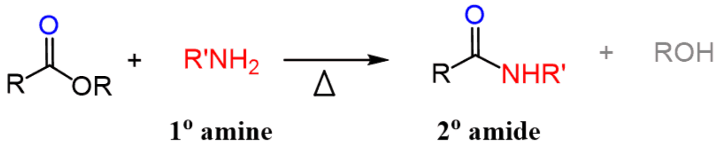
Carboxylic acid **Ammonium carboxylate** **an Amide**

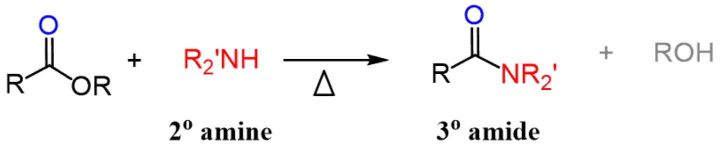


$$R-\overset{O}{\overset{\|}{C}}-OH + R'NH_2 \longrightarrow R-\overset{O}{\overset{\|}{C}}-NHR'+H_2O$$

Carboxylic acid **Primary amine** **Amide (Substituted)**



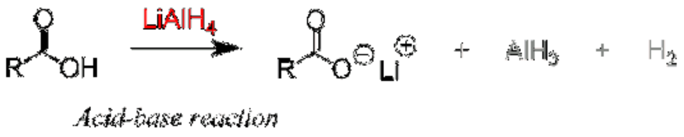


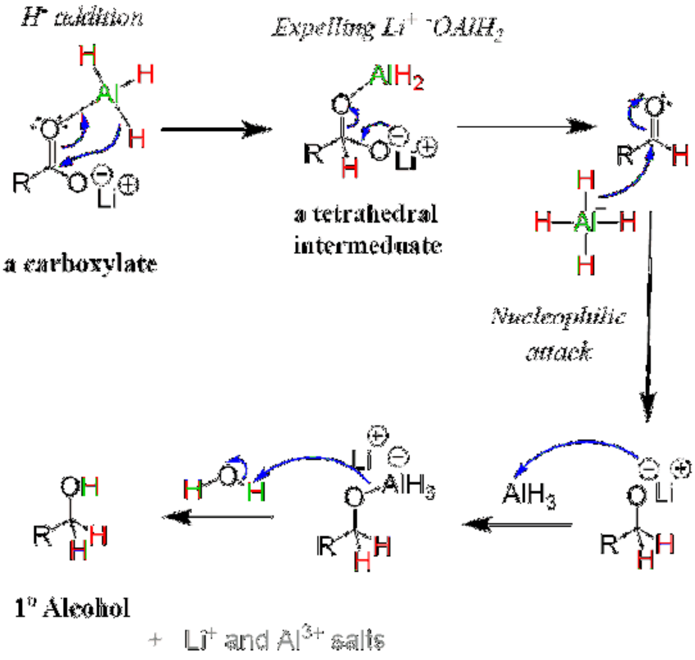


- **Reduction**: Carboxylic acids can be reduced to alcohols.
    - **Example**: Reduction of acetic acid to ethanol.

$$CH_3COOH+2H_2 \rightarrow CH_3CH_2OH+H_2O$$

The Mechanism of Carboxylic Acid Reduction by $LiAlH_4$





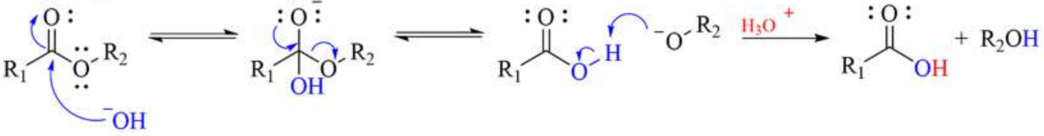
14.2 Derivatives

Carboxylic acids can be converted into various derivatives, which are important in organic chemistry and have diverse applications.

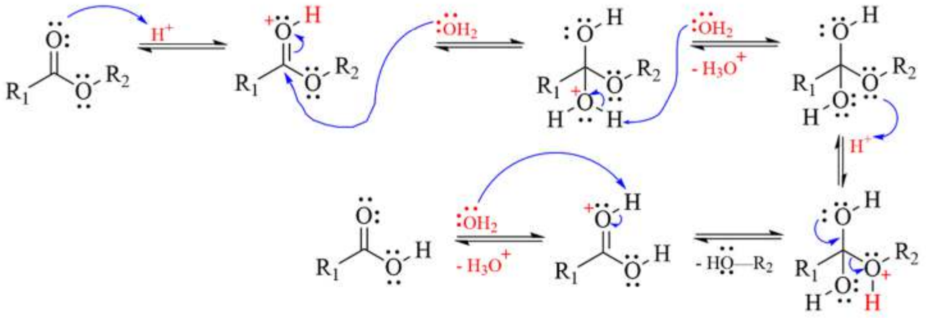
1. **Esters**:
    - **Definition**: Esters are derived from carboxylic acids and alcohols, containing the -COO- group.
    - **General Formula**: R-COO-R', where R and R' can be the same or different alkyl or aryl groups.
    - **Properties**: Esters are generally less polar than carboxylic acids and have pleasant odors.
    - **Examples**:
        - **Ethyl Acetate ($CH_3COOCH_2CH_3$)**: Used as a solvent and in the production of perfumes.
        - **Methyl Benzoate ($C_6H_5COOCH_3$)**: Used in the synthesis of dyes and perfumes.
    - **Reactions**: Esters can undergo hydrolysis to form carboxylic acids and alcohols.
        - **Example**: Hydrolysis of ethyl acetate.

$$CH_3COOCH_2CH_3 + H_2O \rightarrow CH_3COOH + CH_3CH_2OH$$

Base-Catalyzed

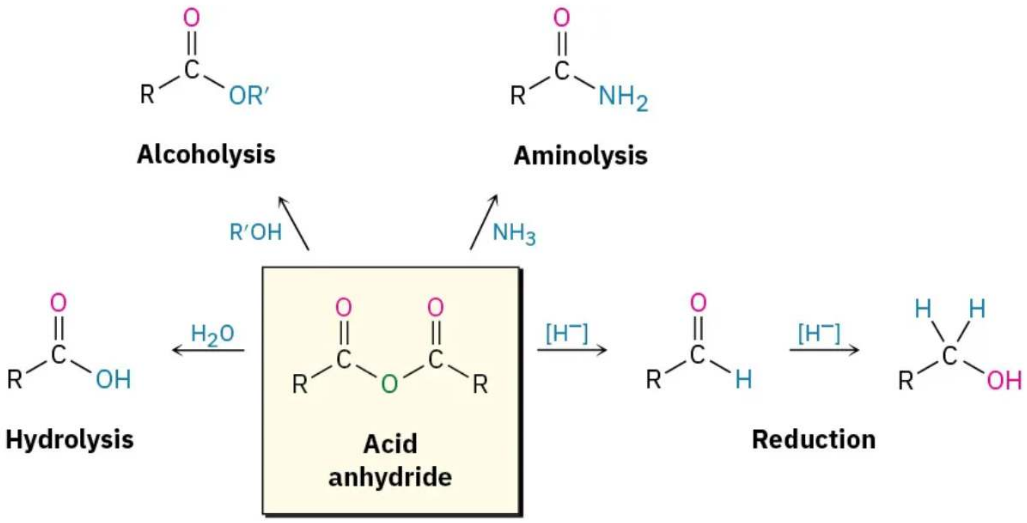


Acid-Catalyzed

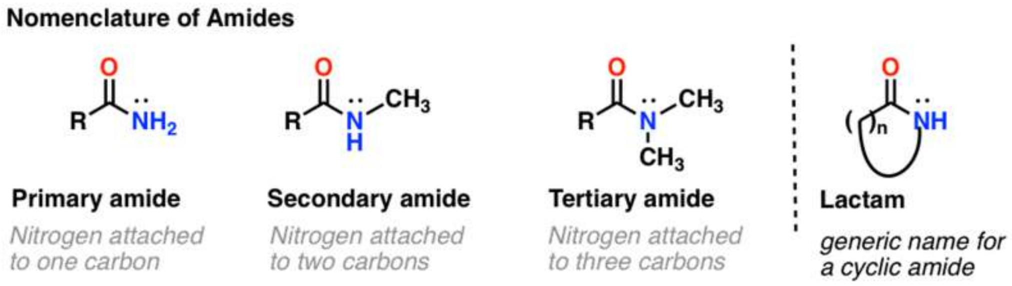


2. **Anhydrides**:
   - **Definition**: Anhydrides are derived from carboxylic acids by the elimination of water, containing the -CO-O-CO- group.
   - **General Formula**: R-CO-O-CO-R’, where R and R’ can be the same or different alkyl or aryl groups.
   - **Properties**: Anhydrides are more reactive than esters and are used as acylating agents.
   - **Examples**:
     - **Acetic Anhydride (CH_3COOCH_3CO)**: Used in the acetylation of alcohols and amines.
   - **Reactions**: Anhydrides can react with alcohols to form esters and with amines to form amides.
     - **Example**: Reaction of acetic anhydride with ethanol.

$CH_3COOCH_3CO+CH_3CH_2OH \rightarrow CH3COOCH_2CH_3+CH_3COOH$

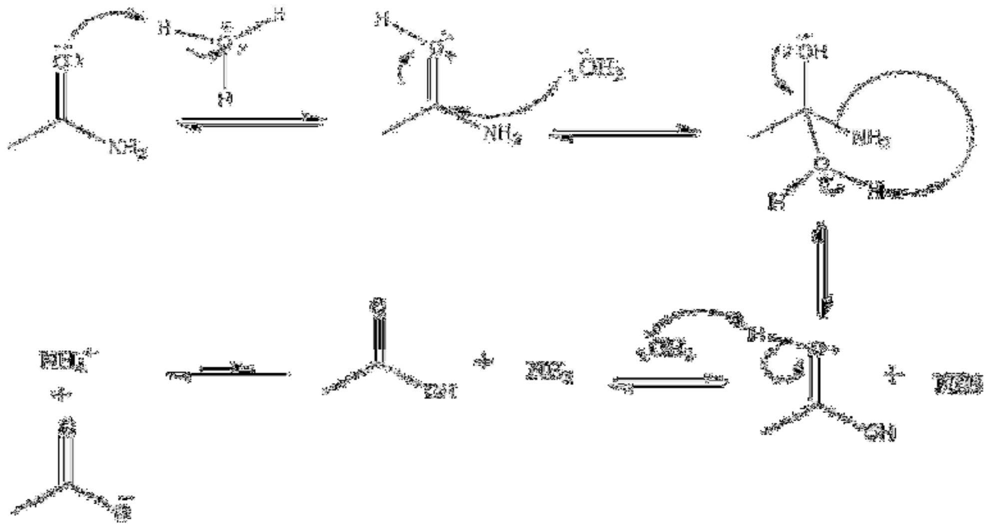


3. **Amides**:
    - **Definition**: Amides are derived from carboxylic acids and amines, containing the -$CONH_2$ group.
    - **General Formula**: R-$CONH_2$, where R can be an alkyl or aryl group.



    - **Properties**: Amides are generally less acidic than carboxylic acids and are more stable to hydrolysis.
    - **Examples**:
        - **Acetamide (CH_3CONH_2)**: Used in the synthesis of other organic compounds.
    - **Reactions**: Amides can undergo hydrolysis to form carboxylic acids and amines.
        - **Example**: Hydrolysis of acetamide.

$$CH_3CONH_2+H_2O \rightarrow CH_3COOH+NH_3$$



14.3 Importance of Carboxylic Acids and Derivatives

Chemical Synthesis:

- **Starting Materials**: Carboxylic acids and their derivatives are commonly used as starting materials in organic synthesis.

- **Functional Group Transformations**: These compounds can undergo various reactions to introduce or transform functional groups.

Biological Systems:

- **Natural Products**: Many natural products, such as amino acids, fatty acids, and nucleic acids, contain carboxylic acid or amide groups.
- **Metabolic Pathways**: Carboxylic acids and their derivatives are intermediates in various metabolic pathways.

Industrial Applications:

- **Solvents**: Esters and anhydrides are used as solvents in various industrial processes.
- **Plastics and Polymers**: Carboxylic acids and their derivatives are used in the production of plastics and polymers.

14.4 Conclusion

Carboxylic acids and their derivatives are important classes of organic compounds with diverse properties and reactivities. Understanding their structures, properties, and reactions is crucial for their application in various fields, including chemical synthesis, biological systems, and industrial processes. The presence of the -COOH, -COO-, -CO-O-CO-, and $-CONH_2$ groups in these compounds influences their reactivity and makes them valuable intermediates in organic chemistry.

Chapter 15: Amines and Amides

15.1 Amines

Amines have an -NH_2 group.

15.2 Amides

Amides have a -$CONH_2$ group.

Example: Ammonia (NH_3)

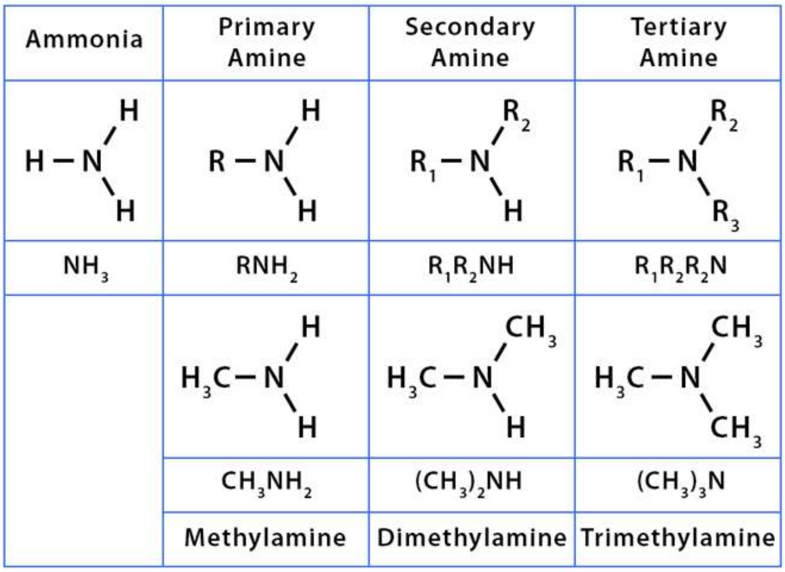
Ammonia is a simple amine with three hydrogen atoms attached to a nitrogen atom.

Chapter 15: Amines and Amides

15.1 Amines

Definition: Amines are organic compounds that contain an -NH_2 group, where the nitrogen atom is bonded to one or more carbon-containing groups. Amines can be classified based on the number of carbon-containing groups attached to the nitrogen atom.
Classification:

- **Primary Amines**: One carbon-containing group is attached to the nitrogen atom (R-NH_2).
    - **Example**: Methylamine (CH_3NH_2)
- **Secondary Amines**: Two carbon-containing groups are attached to the nitrogen atom (R-NHR').
    - **Example**: Dimethylamine (CH_3NHCH_3)
- **Tertiary Amines**: Three carbon-containing groups are attached to the nitrogen atom (R-NR'R'').
    - **Example**: Trimethylamine ($N(CH_3)_3$)



Ammonia	Primary Amine	Secondary Amine	Tertiary Amine
NH_3	RNH_2	R_1R_2NH	$R_1R_2R_2N$
	CH_3NH_2	$(CH_3)_2NH$	$(CH_3)_3N$
	Methylamine	Dimethylamine	Trimethylamine

Properties:

- **Physical State**: Amines with low molecular weights are gases at room temperature, while those with higher molecular weights are liquids or solids.
- **Boiling and Melting Points**: Higher than those of corresponding hydrocarbons due to hydrogen bonding.
- **Solubility**: Soluble in water due to hydrogen bonding with water molecules.
- **Chemical Reactivity**: Amines are basic and can accept protons (H^+) to form ammonium ions.

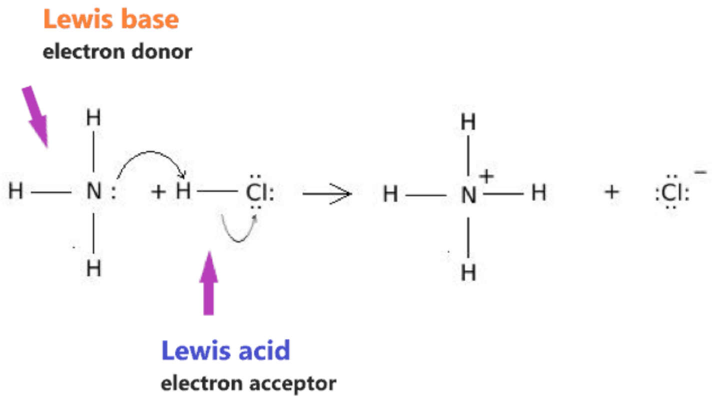
Examples:

- **Ammonia (NH_3)**: The simplest amine, used as a fertilizer and in cleaning products.
- **Methylamine (CH_3NH_2)**: Used in the synthesis of pharmaceuticals and other chemicals.
- **Aniline ($C_6H_5NH_2$)**: An aromatic amine used in the production of dyes and polymers.

Reactions:

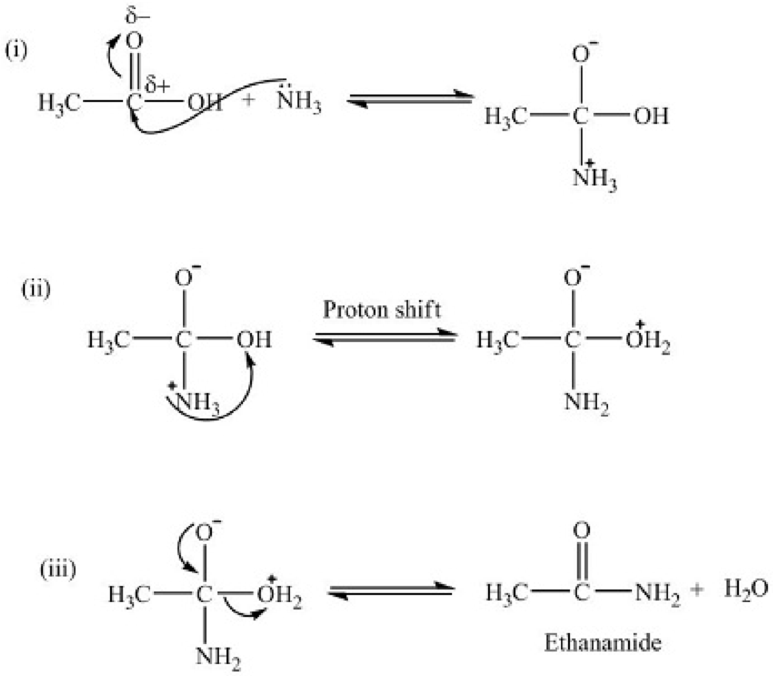
- **Acid-Base Behavior**: Amines can accept protons to form ammonium ions.
  - **Example**: Reaction of ammonia with hydrochloric acid.

    $NH_3+HCl \rightarrow NH_4Cl$



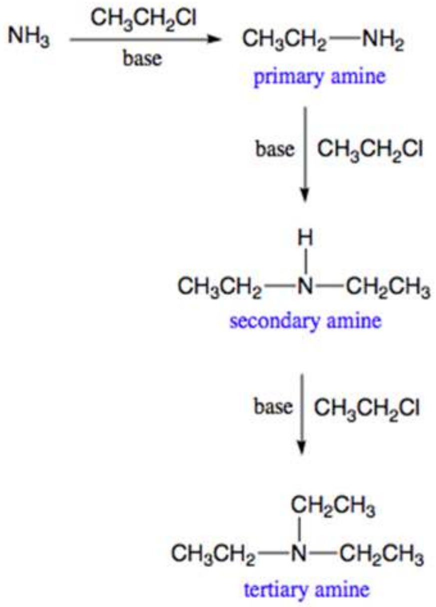
- **Formation of Amides**: Amines can react with carboxylic acids to form amides.
    - **Example**: Reaction of ammonia with acetic acid.

      $NH_3+CH_3COOH \rightarrow CH_3CONH_2+H_2O$



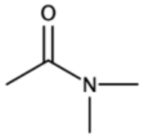
- **Alkylation**: Amines can undergo alkylation reactions to form more complex amines.
    - **Example**: Alkylation of ammonia with ethyl iodide.

      $NH_3+CH_3CH_2I \rightarrow CH_3CH_2NH_2+HI$

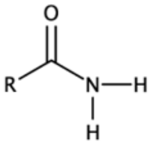


15.2 Amides

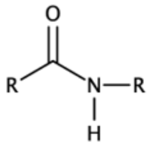
Definition: Amides are organic compounds that contain a $-CONH_2$ group, where the carbonyl group (C=O) is bonded to a nitrogen atom. Amides can be derived from carboxylic acids and amines.
General Formula: The general formula for amides is $R-CONH_2$, where R can be an alkyl or aryl group.



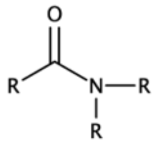
amide functional group



primary amide



secondary amide



tertiary amide

Properties:

- **Physical State**: Amides with low molecular weights are liquids at room temperature, while those with higher molecular weights are solids.
- **Boiling and Melting Points**: Higher than those of corresponding carboxylic acids due to hydrogen bonding.
- **Solubility**: Soluble in water due to hydrogen bonding with water molecules.
- **Chemical Reactivity**: Amides are less reactive than carboxylic acids and amines due to the resonance stabilization of the amide bond.

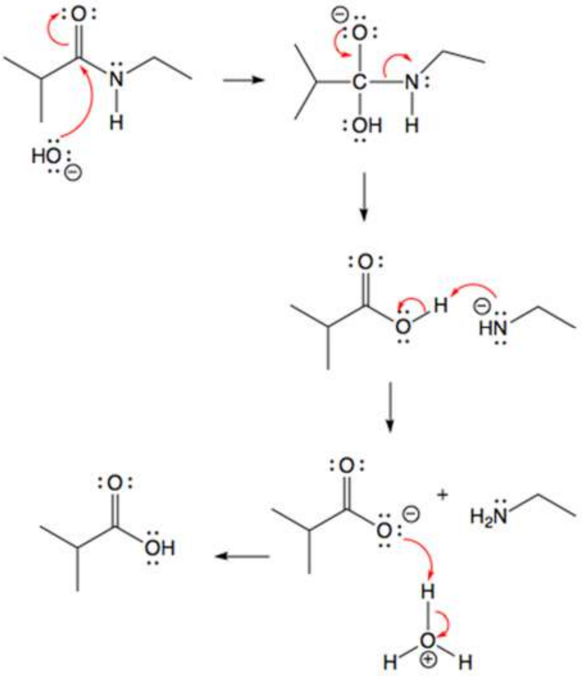
Examples:

- **Acetamide (CH_3CONH_2)**: Used in the synthesis of other organic compounds.
- **Benzoamide ($C_6H_5CONH_2$)**: Used in the production of dyes and pharmaceuticals.
- **Polyamides**: Polymers like nylon, which are composed of repeating amide units.

Reactions:

- **Hydrolysis**: Amides can undergo hydrolysis to form carboxylic acids and amines.
    - **Example**: Hydrolysis of acetamide.

      $CH_3CONH_2 + H_2O \rightarrow CH_3COOH + NH_3$

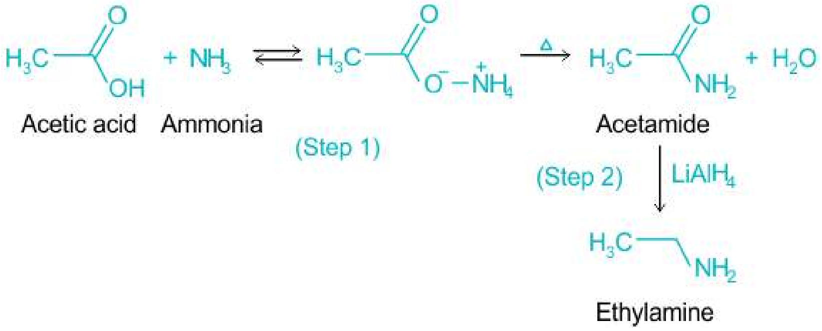


- **Formation**: Amides can be formed by the reaction of carboxylic acids with amines.
    - **Example**: Reaction of acetic acid with ammonia.

      $CH_3COOH + NH_3 \rightarrow CH_3CONH_2 + H_2O$

- **Reduction**: Amides can be reduced to amines.
    - **Example**: Reduction of acetamide to methylamine.

      $CH_3CONH_2 + 2H_2 \rightarrow CH_3NH_2 + H_2O$



15.3 Importance of Amines and Amides

Chemical Synthesis:

- **Starting Materials**: Amines and amides are commonly used as starting materials in organic synthesis.
- **Functional Group Transformations**: These compounds can undergo various reactions to introduce or transform functional groups.

Biological Systems:

- **Natural Products**: Many natural products, such as amino acids, proteins, and nucleic acids, contain amine or amide groups.
- **Pharmaceuticals**: Amines and amides are common functional groups in pharmaceuticals, contributing to their biological activity.

Industrial Applications:

- **Solvents**: Amines are used as solvents in various industrial processes.
- **Polymers**: Amides are used in the production of polymers like nylon and Kevlar.

15.4 Conclusion

Amines and amides are important classes of organic compounds with diverse properties and reactivities. Understanding their structures, properties, and reactions is crucial for their application in various fields, including chemical synthesis, biological systems, and industrial processes. The presence of the $-NH_2$ and $-CONH_2$ groups in these compounds influences their reactivity and makes them valuable intermediates in organic chemistry.

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