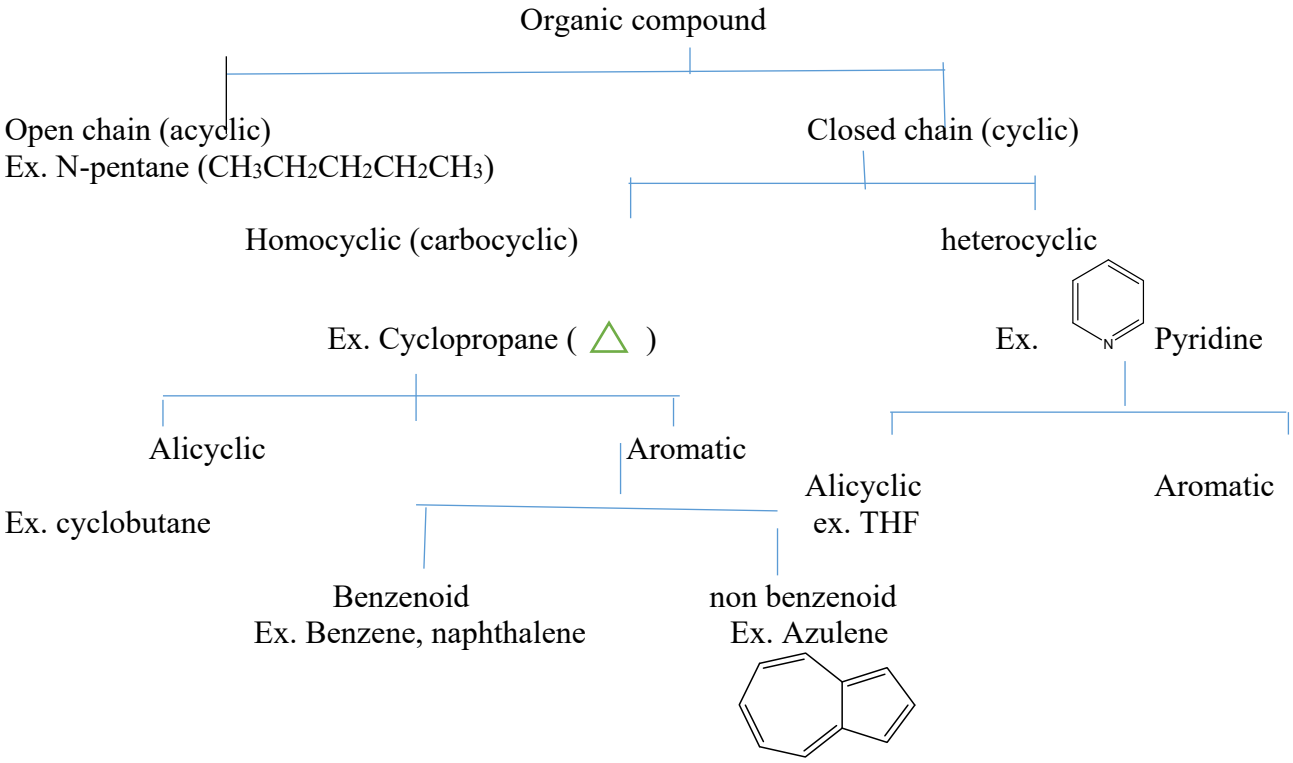
UNIT-I

CLASSIFICATION AND NOMENCLATURE OF ORGANIC COMPOUND



Short Summary of IUPAC Nomenclature of Organic Compounds

Introduction

- The purpose of the IUPAC system of nomenclature is to establish an international standard of naming compounds to facilitate communication.

I. Fundamental Principle

- IUPAC nomenclature is based on naming a molecule's longest chain of carbons connected by single bonds, whether in a continuous chain or in a ring.
- All deviations, either multiple bonds or atoms other than carbon and hydrogen, are indicated by prefixes or suffixes according to a specific set of priorities.

II. Alkanes and Cycloalkanes

- Alkanes are the family of saturated hydrocarbons, that is, molecules containing carbon and hydrogen connected by single bonds only.
- These molecules can be in continuous chains (called linear or acyclic), or in rings (called cyclic or alicyclic).
- The names of alkanes and cycloalkanes are the root names of organic compounds. Beginning with the five-carbon alkane, the number of carbons in the chain is indicated by the Greek or Latin prefix.
- Rings are designated by the prefix "cyclo". (In the geometrical symbols for rings, each apex represents a carbon with the number of hydrogens required to fill its valence.)

CH_4	methane	$CH_3[CH_2]_{10}CH_3$	dodecane
CH_3CH_3	ethane	$CH_3[CH_2]_{11}CH_3$	tridecane
$CH_3CH_2CH_3$	propane	$CH_3[CH_2]_{12}CH_3$	tetradecane
$CH_3[CH_2]_2CH_3$	butane	$CH_3[CH_2]_{18}CH_3$	icosane

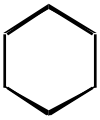
$CH_3[CH_2]_3CH_3$	pentane
$CH_3[CH_2]_4CH_3$	hexane
$CH_3[CH_2]_5CH_3$	heptane
$CH_3[CH_2]_6CH_3$	octane
$CH_3[CH_2]_7CH_3$	nonane
$CH_3[CH_2]_8CH_3$	decane
$CH_3[CH_2]_9CH_3$	undecane

$CH_3[CH_2]_{19}CH_3$	henicosane
$CH_3[CH_2]_{20}CH_3$	docosane
$CH_3[CH_2]_{21}CH_3$	tricosane
$CH_3[CH_2]_{28}CH_3$	triacontane
$CH_3[CH_2]_{29}CH_3$	hentriacontane
$CH_3[CH_2]_{38}CH_3$	tetracontane
$CH_3[CH_2]_{48}CH_3$	pentacontane

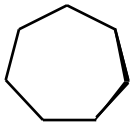
cyclopropane

cyclobutane

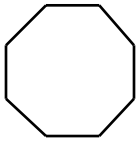
cyclopentane



cyclohexane



cycloheptane



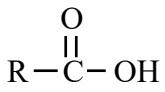
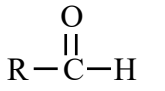
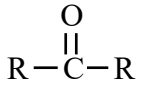
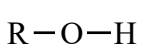
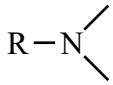
cyclooctane

III. Nomenclature of Molecules Containing Substituents and Functional Groups

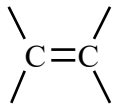
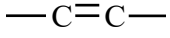
A. Priorities of Substituents and Functional Groups

- LISTED HERE FROM HIGHEST TO LOWEST PRIORITY, except that the substituents within Group C have equivalent priority.

Group A—Functional Groups Indicated By Prefix Or Suffix

Family of Compound	Structure	Prefix	Suffix
Carboxylic Acid		carboxy-	-oic acid (-carboxylic acid)
Aldehyde		oxo- (formyl)	-al (carbaldehyde)
Ketone		oxo-	-one
Alcohol		hydroxy-	-ol
Amine		amino-	-amine

Group B—Functional Groups Indicated By Suffix Only

Family of Compound	Structure	Prefix	Suffix
Alkene		--------	-ene
Alkyne		--------	-yne

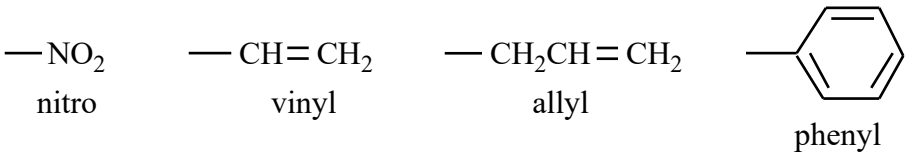
Group C—Substituents Indicated by Prefix Only

Substituent	Structure	Prefix	Suffix
Alkyl (see list below)	R—	alkyl-	----------
Alkoxy	R— O —	alkoxy-	----------
Halogen	F —	fluoro-	----------
	Cl —	chloro-	----------
	Br —	bromo-	----------
	I —	iodo-	----------

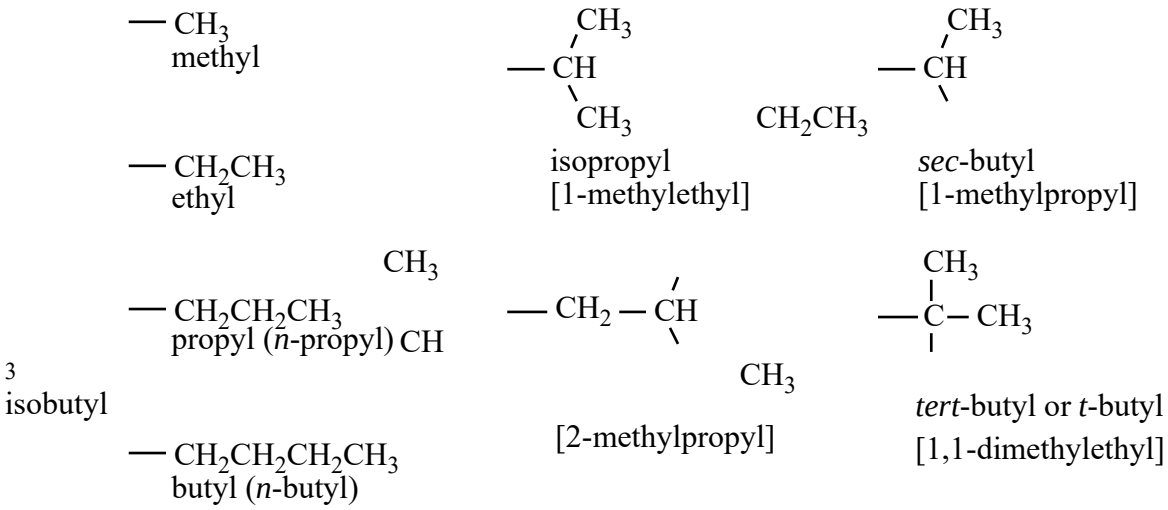
Group C continued on next page

Group C—Substituents, continued

Miscellaneous substituents and their prefixes



Common alkyl groups—replace "ane" ending of alkane name with "yl". Alternate names for complex substituents are given in brackets.



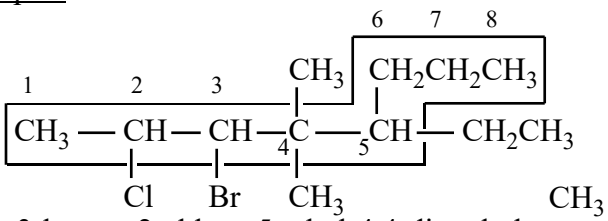
B. Naming Substituted Alkanes and Cycloalkanes—Group C Substituents Only

1. Organic compounds containing substituents from Group C are named following this sequence of steps, as indicated on the examples below:

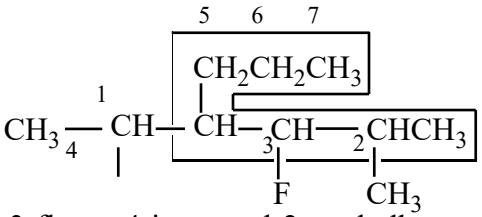
- **Step 1.** Find the longest continuous carbon chain. Determine the root name for this parent chain. In cyclic compounds, the ring is usually considered the parent chain, unless it is attached to a longer chain of carbons; indicate a ring with the prefix "cyclo" before the root name. (When there are two longest chains of equal length, use the chain with the greater number of substituents.)
- **Step 2.** Number the chain in the direction such that the position number of the first substituent is the smaller number. If the first substituents from either end have the same number, then number so that the second substituent has the smaller number, *etc*.
- **Step 3.** Determine the name and position number of each substituent. (A substituent on a nitrogen is designated with an "*N*" instead of a number.
- **Step 4.** Indicate the number of identical groups by the prefixes di, tri, tetra, *etc*.
- **Step 5.** Place the position numbers and names of the substituent groups, in alphabetical order, before the root name. In alphabetizing, ignore prefixes like *sec*-, *tert*-, di, tri, *etc*., but include iso and cyclo. Always include a position number for each substituent.

Short Summary of IUPAC Nomenclature,

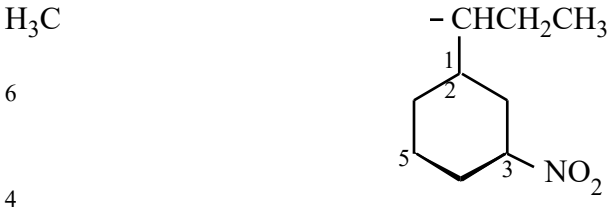
Examples



3-bromo-2-chloro-5-ethyl-4,4-dimethyloctane



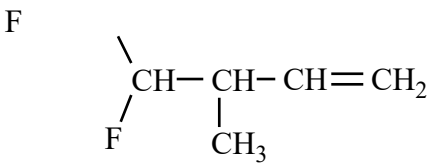
3-fluoro-4-isopropyl-2-methylheptane



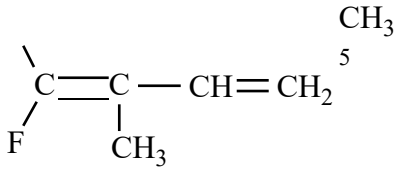
1-*sec*-butyl-3-nitrocyclohexane (numbering determined by the alphabetical order of substituents)

C. **Naming Molecules Containing Functional Groups from Group B—Suffix Only**

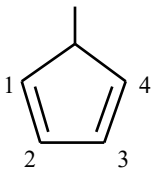
1. **Alkenes**—Follow the same steps as for alkanes, except:
   a. Number the chain of carbons *that includes the C=C* so that the C=C has the lower position number, since it has a higher priority than any substituents;
   b. Change "ane" to "ene" and assign a position number to the first carbon of the C=C;
   c. Designate geometrical isomers with a *cis,trans* or *E,Z* prefix.



4,4-difluoro-3-methylbut-1-ene



1,1-difluoro-2-methyl-buta-1,3-diene



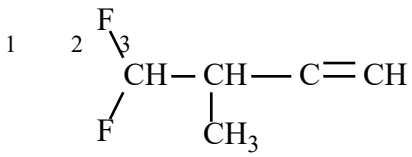
5-methylcyclopenta-1,3-diene

Special case: When the chain cannot include the C=C, a substituent name is used.

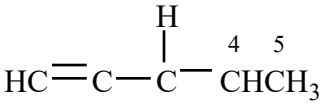
3-vinylcyclohex-1-ene

2. **Alkynes**—Follow the same steps as for alkanes, except:
   a. Number the chain of carbons *that includes the C≡C* so that the functional group has the lower position number;
   b. Change "ane" to "yne" and assign a position number to the first carbon of the C≡C.

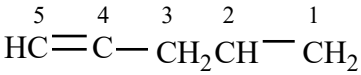
Note: The Group B functional groups (alkene and alkyne) are considered to have equal priority: in a molecule with both a double and a triple bond, whichever is closer to the end of the chain determines the direction of numbering. In the case where each would have the same position number, the double bond takes the lower number. In the name, "ene" comes before "yne" because of alphabetization. See examples on next page.



4,4-difluoro-3-methylbut-1-yne



pent-3-en-1-yne
("yne" closer to end of chain)



pent-1-en-4-yne
("ene" and "yne" have equal priority unless they have the same position number, when "ene" takes the lower number)

(Notes: 1. An “e” is dropped if the letter following it is a vowel: “pent-3-en-1-yne” , not “3-pent-3-ene-1-yne”. 2. An “a” is added if inclusion of di, tri, *etc*., would put two consonants consecutively: “buta-1,3-diene”, not “but-1,3-diene”.)

D. **Naming Molecules Containing Functional Groups from Group A—Prefix or Suffix**

In naming molecules containing one or more of the functional groups in Group A, the group of highest priority is indicated by suffix; the others are indicated by prefix, with priority equivalent to any other substituents. The table in Section **III**.A. defines the priorities; they are discussed below in order of increasing priority.

Now that the functional groups and substituents from Groups A, B, and C have been described, a modified set of steps for naming organic compounds can be applied to all simple structures:

•Step 1. Find the highest priority functional group. Determine and name the longest continuous carbon chain that includes this group.

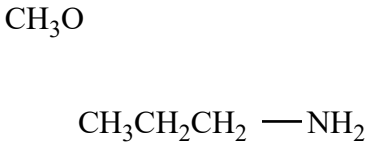
•Step 2. Number the chain so that the highest priority functional group is assigned the lower number.

•Step 3. If the carbon chain includes multiple bonds (Group B), replace “ane” with “ene” for an alkene or “yne” for an alkyne. Designate the position of the multiple bond with the number of the first carbon of the multiple bond.

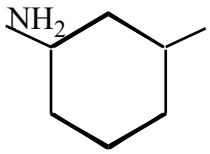
•Step 4. If the molecule includes Group A functional groups, replace the last “e” with the suffix of the highest priority functional group, and include its position number.

•Step 5. Indicate all Group C substituents, and Group A functional groups of lower priority, with a prefix. Place the prefixes, with appropriate position numbers, in alphabetical order before the root name.

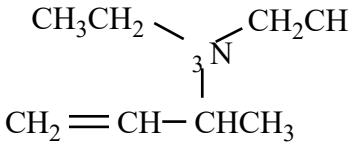
1. Amines: prefix: amino-; suffix: -amine—substituents on nitrogen denoted by “*N*”



propan-1-amine



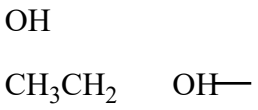
3-methoxycyclohexan-1-amine
("1" is optional in this case)



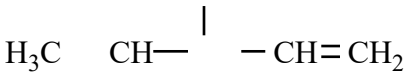
N,*N*-diethylbut-3-en-2-amine

Short Summary of IUPAC Nomenclature,

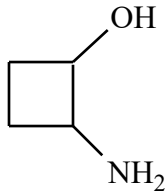
2. Alcohols: prefix: hydroxy-; suffix: -ol



ethanol

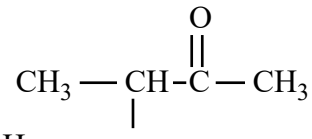


but-3-en-2-ol

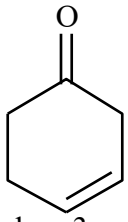


2-aminocyclobutan-1-ol
("1" is optional in this case)

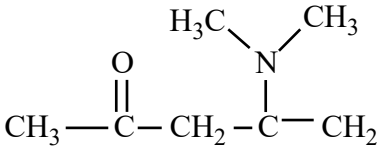
3. Ketones: prefix: oxo-; suffix: -one



3-hydroxybutan-2-one

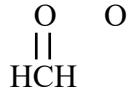


cyclohex-3-en-1-one
("1" is optional in this case)

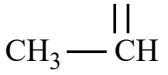


4-(*N*,*N*-dimethylamino)pent-4-en-2-one

4. Aldehydes: prefix: oxo-, or formyl- (O=CH-); suffix: -al (abbreviation: —CHO).
An aldehyde can only be on carbon 1, so the "1" is generally omitted from the name.

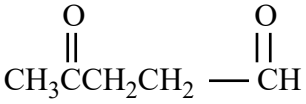


methanal;
formaldehyde



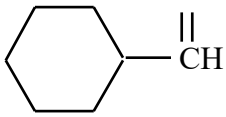
ethanal;
acetaldehyde

4-hydroxybut-2-enal



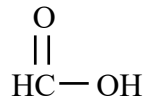
4-oxopentanal

Special case: When the chain cannot include the carbon of the CHO, the suffix "carbaldehyde" is used:

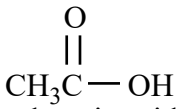


cyclohexanecarbaldehyde

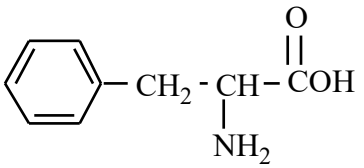
5. Carboxylic Acids: prefix: carboxy-; suffix: -oic acid (abbreviation: —COOH).
A carboxylic acid can only be on carbon 1, so the "1" is generally omitted from the name.



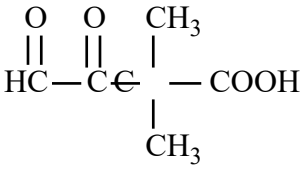
methanoic acid;
formic acid



ethanoic acid;
acetic acid



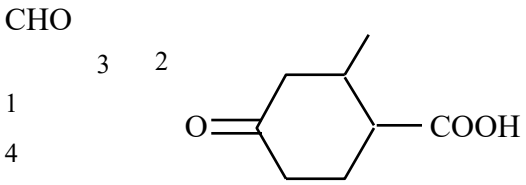
2-amino-3-phenylpropanoic acid



2,2-dimethyl-3,4-dioxobutanoic acid

(Note: Chemists traditionally use, and IUPAC accepts, the names "formic acid" and "acetic acid" in place of "methanoic acid" and "ethanoic acid".)

Special case: When the chain numbering cannot include the carbon of the COOH, the suffix "carboxylic acid" is used. See example on next page.



2-formyl-4-oxocyclohexanecarboxylic acid ("formyl" is used to indicate an aldehyde as a substituent when its carbon cannot be in the chain numbering)

E. **Naming Carboxylic Acid Derivatives**

The six common groups derived from carboxylic acids are salts, anhydrides, esters, acyl halides, amides, and nitriles. Salts and esters are most important.

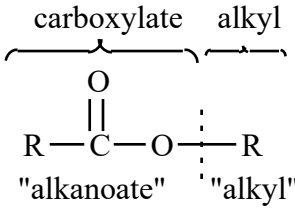
1. Salts of Carboxylic Acids

Salts are named with cation first, followed by the anion name of the carboxylic acid, where "**ic acid**" is replaced by "**ate**" :

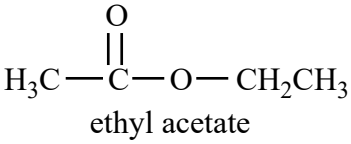
acet**ic acid**	becomes	acet**ate**
butano**ic acid**	becomes	butano**ate**
cyclohexanecarboxyl**ic acid**	becomes	cyclohexanecarboxyl**ate**

2. **Esters**

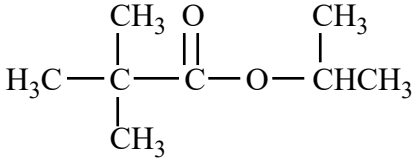
Esters are named as "organic salts" that is, the alkyl name comes first, followed by the name of the carboxylate anion. (common abbreviation: —COOR)



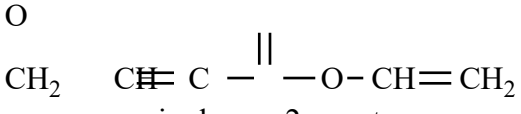
"alkyl alkanoate"



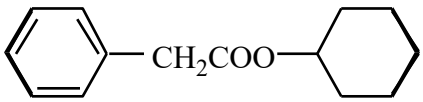
ethyl acetate



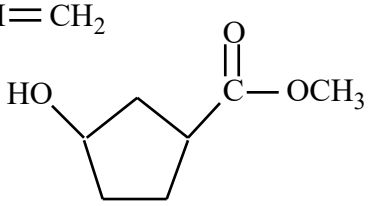
isopropyl 2,2-dimethylpropanoate



vinyl prop-2-enoate



cyclohexyl 2-phenylacetate



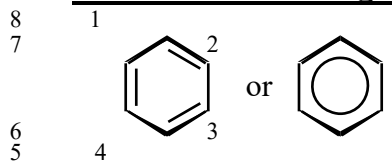
methyl 3-hydroxycyclopentanecarboxylate

IV. Nomenclature of Aromatic Compounds

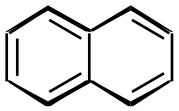
"Aromatic" compounds are those derived from benzene and similar ring systems. As with aliphatic nomenclature described above, the process is: determining the root name of the parent ring; determining priority, name, and position number of substituents; and assembling the name in alphabetical order. *Functional group priorities are the same in aliphatic and aromatic nomenclature.*

Short Summary of IUPAC Nomenclature,

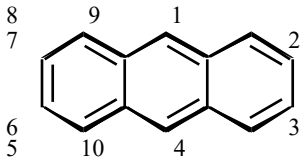
A. **Common Parent Ring Systems**



benzene



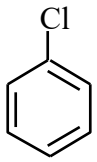
naphthalene



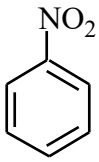
anthracene

B. **Monosubstituted Benzenes**

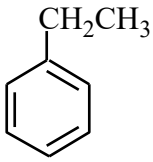
1. Most substituents keep their designation, followed by the word "benzene":



chlorobenzene

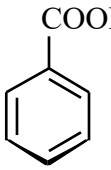


nitrobenzene

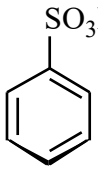


ethylbenzene

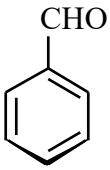
2. Some common substituents change the root name of the ring. IUPAC accepts these as root names, listed here in decreasing priority:



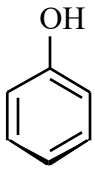
benzoic acid



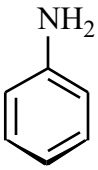
benzene-sulfonic acid



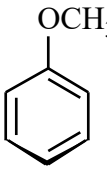
benzaldehyde



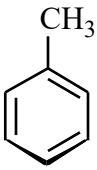
phenol



aniline



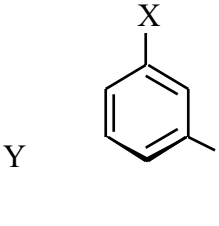
anisole

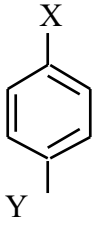


toluene

C. **Disubstituted Benzenes**

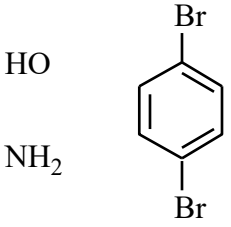
1. Designation of substitution—only three possibilities:



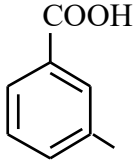


common:	*ortho-*	*meta-*	*para-*
IUPAC:	1,2-	1,3-	1,4-

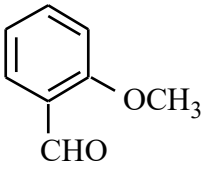
2. Naming disubstituted benzenes—Priorities determine root name and substituents



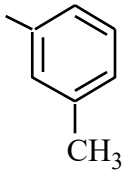
1,4-dibromobenzene



3-aminobenzoic acid



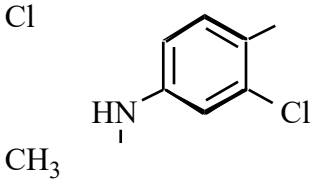
2-methoxybenzaldehyde



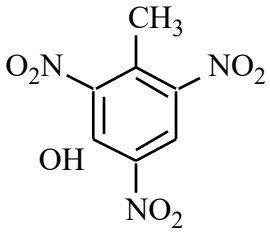
3-methylphenol

Short Summary of IUPAC Nomenclature,

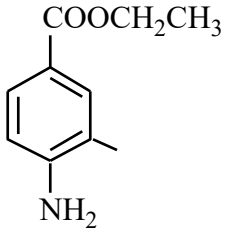
D. Polysubstituted Benzenes



3,4-dichloro-*N*-methylaniline



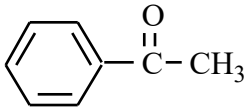
2,4,6-trinitrotoluene (TNT)



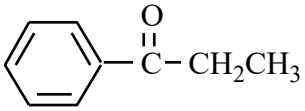
ethyl 4-amino-3-hydroxybenzoate

E. Aromatic Ketones

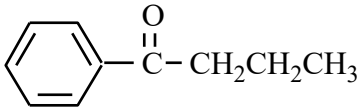
A special group of aromatic compounds are ketones where the carbonyl is attached to at least one benzene ring. Such compounds are named as "phenones", the prefix depending on the size and nature of the group on the other side of the carbonyl. These are the common examples:



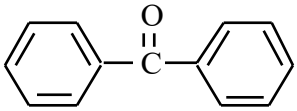
acetophenone



propiophenone



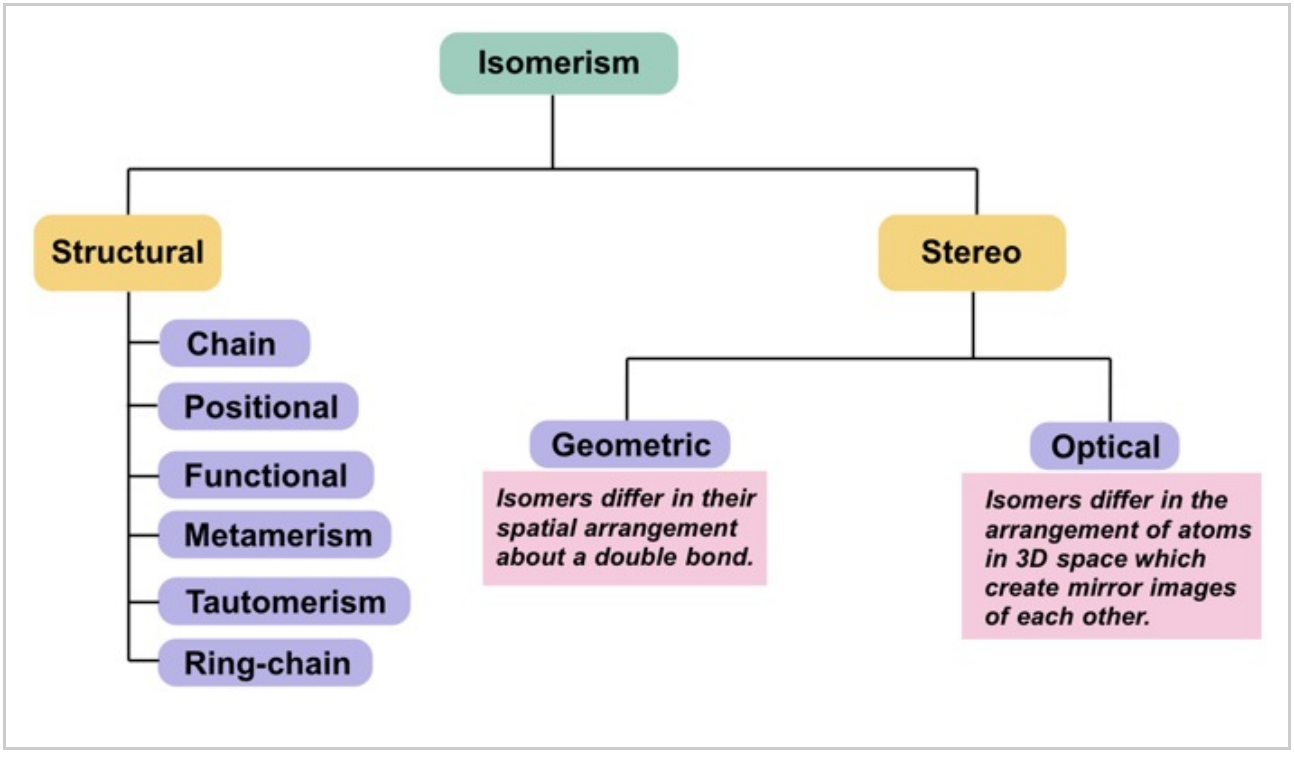
butyrophenone



benzophenone

Introduction

Isomerism in organic chemistry is a phenomenon shown by two or more organic compounds having the same molecular formula but different properties due to difference in arrangement of atoms along the carbon skeleton (structural isomerism) or in space (Stereo isomerism). The chart summarizes the types of isomerism, and we will discuss only ***structural isomerism*** in greater detail.



Structural Isomerism

Chain Isomerism

It occurs when carbon atoms are linked to the main chain in different ways. For example:

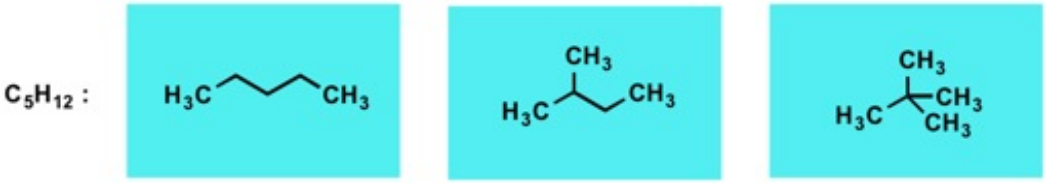


Figure 2. Pentane chain isomers

Position Isomerism

It occurs when functional groups are attached on different positions on a carbon chain. For example:

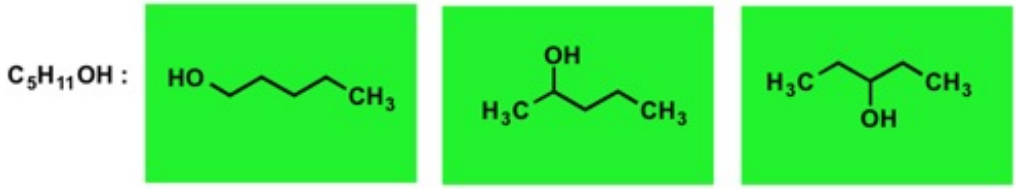


Figure 3. Position isomerism

Functional Isomerism

It is a very interesting form of isomerism where the compounds are different due to different arrangements of atoms leading to different functional groups. As functional groups are usually the reactive centre of a molecule this leads to entirely different properties. For example:

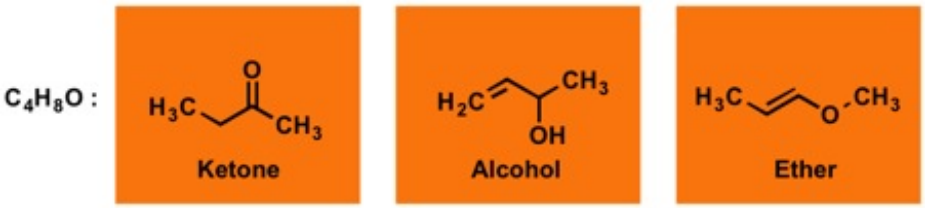


Figure 4. Functional isomerism

Metamerism

This form of isomerism is rare and is limited to molecules having a divalent atom like O or S and alkyl groups around it. The main examples come from ethers and thioethers.

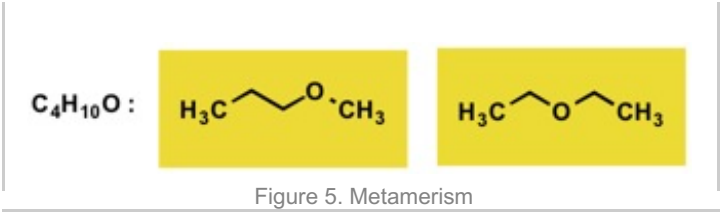


Figure 5. Metamerism

Tautomerism

This isomerism is due to spontaneous intreconversion of two isomeric forms with different functional groups. The prerequisites for this is the presence of the C=O, C==N or N=O in the usual cases and an alpha H atom. The most usual is the ‘keto-enol’ tautomerism, but there can be others like nitro-aci and amine-imine forms.

In general the Keto form is more stable. Enols can be forms by acid or base catalysis from the ketone and are extensively used in making C-C single bonds in organic synthesis.

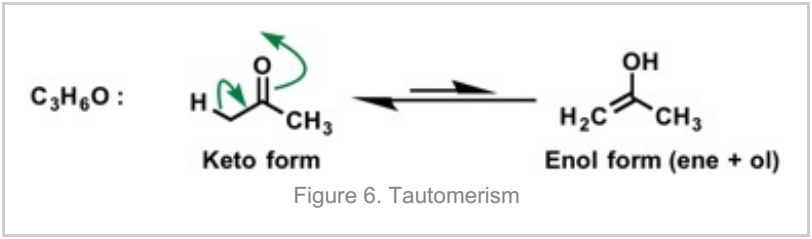


Figure 6. Tautomerism

Ring-Chain isomerism

Here one isomer is an open chain molecule and the other a cyclic molecule.

Propene is an alkene and cyclopropane an alkane, two different classes of compounds.

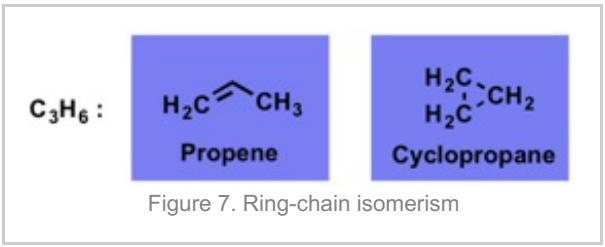


Figure 7. Ring-chain isomerism