

IUPAC Naming of Organic Compounds with Functional Groups

With the ability to identify functional groups, next we will learn how to give IUPAC names to compounds containing several functional groups by following a set of rules.

IUPAC NOMENCLATURE of COMPOUNDS with FUNCTIONAL GROUPS

1. Find the longest carbon chain containing the functional group with the highest priority (see **Table 2.3**). This chain determines the *parent name* of the compound.
2. Change the ending of the parent alkane/alkene/alkyne to the *suffix* of the highest priority group, which gives the parent name of the compound (usually, drop the last letter “e” before adding the suffix, except for nitrile where the “e” is kept).
3. Number the chain from the end closest to the highest functional group.
4. The other groups are named as substituents by using the appropriate *prefixes*.
5. Assign stereochemistry, E/Z or R/S, as necessary (details in **Chapter 5**).

For naming purposes, the functional groups are assigned with priorities (Table 2.3). If the compound includes more than one functional group, the one with the *highest* priority is the “parent structure” and determines the “parent name”; the other groups will be regarded as “substituents”. The “suffix” is used to indicate the name of the parent structure, and the “prefix” is for the substituent. The order of the groups listed in **Table 2.3** is based on the *decreasing* order of priority, where the carboxylic acid group is in the highest priority. The groups in the subordinate table have no difference in terms of priority, and they are usually listed in alphabetic order.

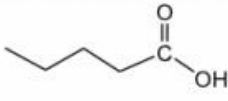
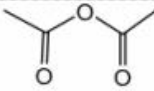
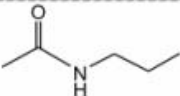
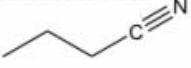
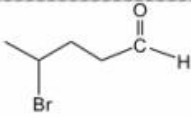
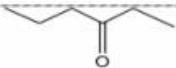
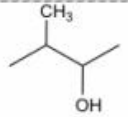


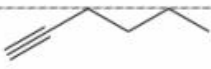


Functional group	Prefix	Suffix	Examples	Name of Example
carboxylic acid	carboxy	-oic acid -carboxylic acid		pentanoic acid
acid anhydride	—	-oic anhydride -carboxylic anhydride		ethanoic anhydride
carboxylic ester	alkoxycarbonyl	-oate -carboxylate	$\text{CH}_3\text{CH}_2\text{C}(=\text{O})\text{OCH}_3$	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)
alkene	enyl	-ene		2-pentene
alkyne	ynyl	-yne		1-hexyne
alkyl	yl	-ane		2,2-dimethylbutane

Table 2.3 Naming Priorities of Common Functional Groups

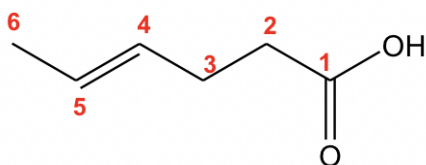
Functional group	Structure	Prefix	Suffix
alkyl halide	R—X (X: F, Br, Cl, I)	halo (fluoro, bromo, chloro, iodo)	—
ether	R—O—R	oxy	ether
sulfide	R—S—R	alkylthio	sulfide
nitro	—NO ₂	nitro	—
benzene		phenyl	benzene

Table

2.4 Subordinate Groups

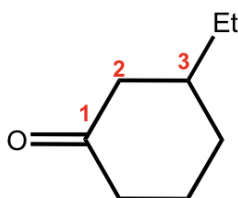
We will go through several examples for more details about the naming rules.

1.



The parent structure is the 6-carbon carboxylic acid with a double bond, so the last name comes from “hexene”. To add the suffix, the last letter “e” will be dropped, so the parent name is “hexeneoicacid”. A number is necessary to indicate the position of the double bond, so the name is “4-hexeneoic acid”. The carboxylic acid group is always in the #1 position, so it is NOT necessary to include that number for the position.

2.



This is a ketone based on a cycloalkane, so the last name comes from “cyclohexane”. By adding the suffix, it becomes “cyclohexanone”, and the complete name is “3-ethylcyclohexanone”.

Homologous series:

- A homologous series is a collection of compounds with the same general formula that differ only in the carbon chain length.
- Compounds in a homologous series often have a fixed set of functional groups, resulting in chemical and physical properties that are comparable.
- For example, homologous series of alkane: CH_4 , C_2H_6 , C_3H_8 , etc. are homologous.
- They differ from each other by $-\text{CH}_2$ unit.

The characteristics of homologous series:

- The functional group of the members of the homologous series is the same.
- The general formula is the same for all members.
- Members of homologous series have nearly identical chemical properties due to the same functional group.
- Members of homologous series have a general method of preparation in common.

What is Isomerism?

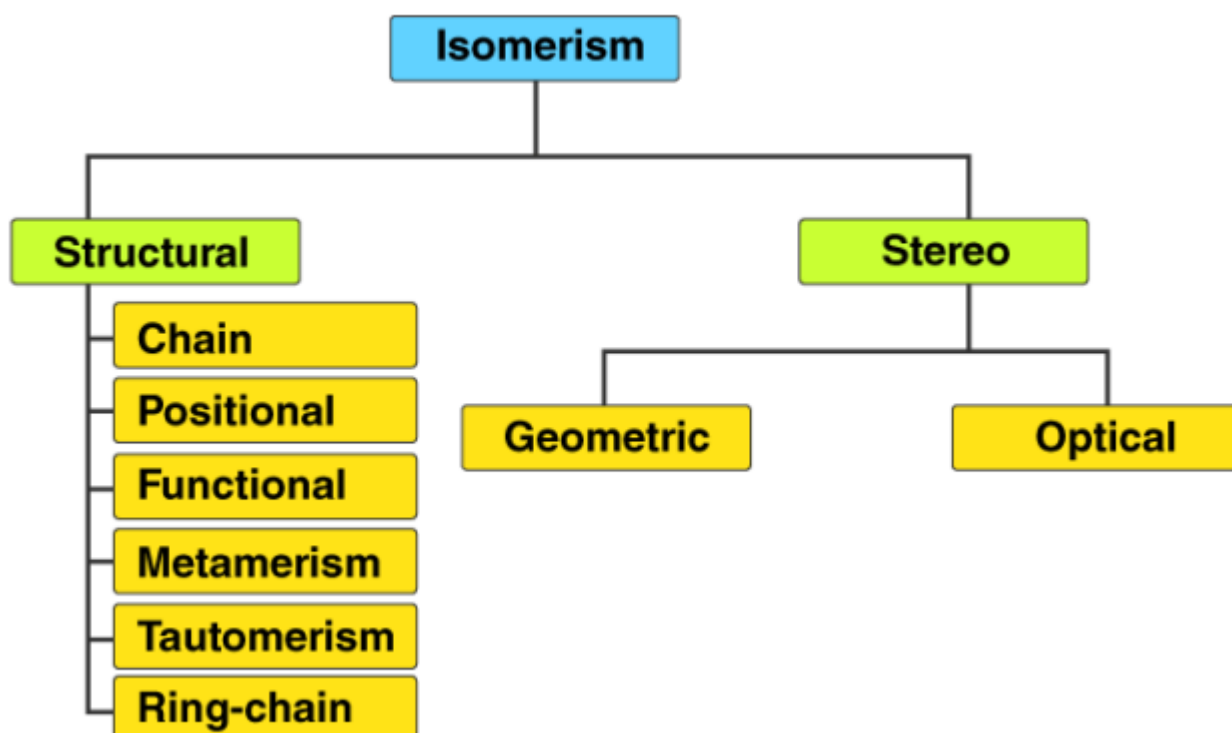
Isomerism is the phenomenon in which more than one compounds have the same chemical formula but different chemical structures.

Chemical compounds that have identical chemical formulae but differ in properties and the arrangement of atoms in the molecule are called **isomers**. Therefore, the compounds that exhibit isomerism are known as isomers.

The word "isomer" is derived from the Greek words "isos" and "meros", which mean "equal parts". This term was coined by the Swedish chemist Jacob Berzelius in the year 1830.

Isomerism Types

There are two primary types of isomerism, which can be further categorized into different subtypes. These primary types are **Structural Isomerism** and **Stereoisomerism**. The classification of different types of isomers is illustrated below.



Structural Isomerism

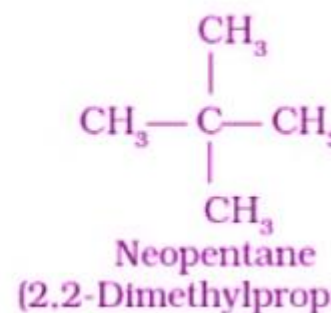
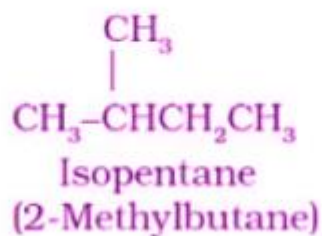
Structural isomerism is commonly referred to as constitutional isomerism. The functional groups and the atoms in the molecules of these isomers are linked in different ways. Different structural isomers are assigned different IUPAC names since they may or may not contain the same functional group.

The different types of structural isomerism are discussed in this subsection.

Chain Isomerism

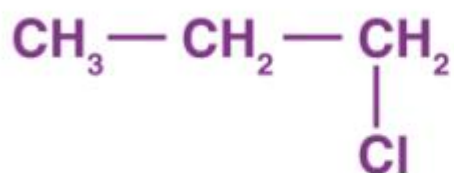
- It is also known as skeletal isomerism.
- The components of these isomers display differently branched structures.
- Commonly, chain isomers differ in the branching of [carbon](#)

- An example of chain isomerism can be observed in the compound C_5H_{12} , as illustrated below.

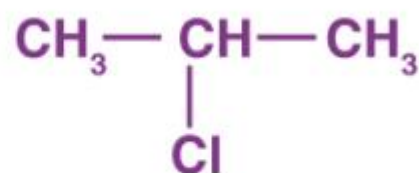


Position Isomerism

- The positions of the functional groups or substituent atoms are different in position isomers.
- Typically, this isomerism involves the attachment of the functional groups to different carbon atoms in the carbon chain.
- An example of this type of isomerism can be observed in the compounds having the formula C_3H_7Cl .



1-Chloropropane

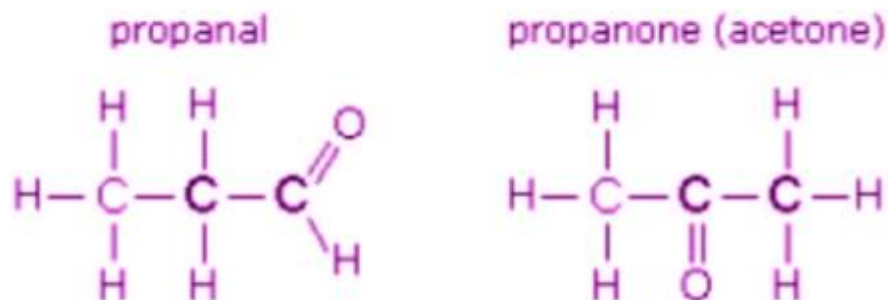


2-Chloropropane

Functional Isomerism

- It is also known as functional group isomerism.
- As the name suggests, it refers to the compounds that have the same chemical formula but different [functional groups](#) attached to them.

- An example of functional isomerism can be observed in the compound C_3H_6O .



Metamerism

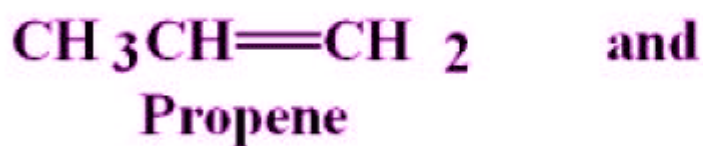
- This type of isomerism arises due to the presence of different alkyl chains on each side of the functional group.
- It is a rare type of isomerism and is generally limited to molecules that contain a divalent atom (such as sulphur or oxygen), surrounded by alkyl groups.
- Example: $C_4H_{10}O$ can be represented as ethoxyethane ($C_2H_5OC_2H_5$) and methoxypropane ($CH_3OC_3H_7$).

Tautomerism

- A tautomer of a compound refers to the isomer of the compound which only differs in the position of protons and electrons.
- Typically, the tautomers of a compound exist together in equilibrium and easily interchange.
- It occurs via an intramolecular proton transfer.
- An important example of this phenomenon is Keto-enol tautomerism.

Ring-Chain Isomerism

- In ring-chain isomerism, one of the isomers has an open-chain structure whereas the other has a ring structure.
- They generally contain a different number of pi bonds.
- A great example of this type of isomerism can be observed in C_3H_6 . Propene and cyclopropane are the resulting isomers, as illustrated below.

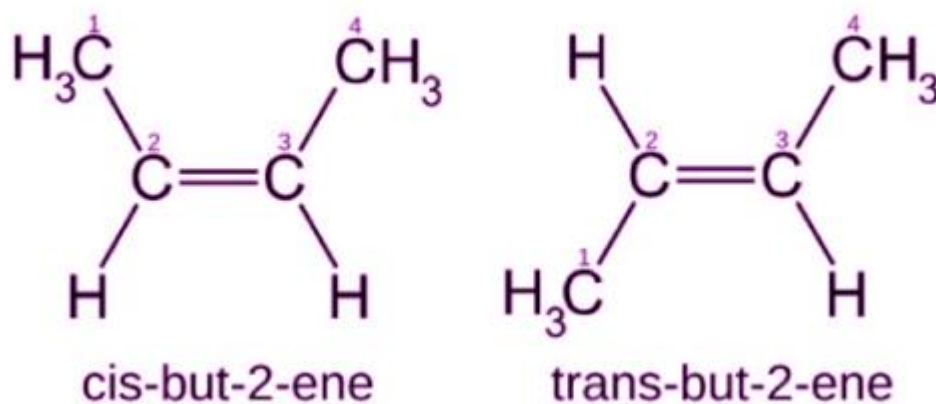


Stereoisomerism

This type of isomerism arises in compounds having the same chemical formula but different orientations of the atoms belonging to the molecule in three-dimensional space. The compounds that exhibit stereoisomerism are often referred to as stereoisomers. This phenomenon can be further categorized into two subtypes. Both these subtypes are briefly described in this subsection.

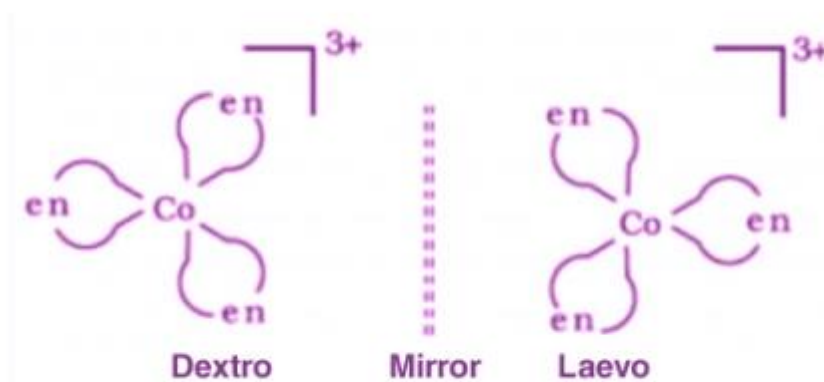
Geometric Isomerism

- It is popularly known as [cis-trans isomerism](#).
- These isomers have different spatial arrangements of atoms in three-dimensional space.
- An illustration describing the geometric isomerism observed in the acyclic But-2-ene molecule is provided below.



Optical Isomerism

- Compounds that exhibit optical isomerism feature similar bonds but different spatial arrangements of atoms forming non-superimposable mirror images.
- These optical isomers are also known as enantiomers.
- Enantiomers differ from each other in their optical activities.
- Dextro enantiomers rotate the plane of polarized light to the right whereas laevo enantiomers rotate it to the left, as illustrated below.



What is Conformation?

In alkanes, the distribution of electrons in a sigma molecular orbital is symmetrical around the internuclear axis of the C-C bond. Thus, it permits the possibility of free rotation about the C-C single bond. Due to this rotation, different spatial arrangements of carbon atoms in space are observed which can change into one another. Such spatial arrangement of carbon and hydrogen atoms which can be converted into one another by rotation around a C-C single bond is called conformation or conformer or rotamer. [Alkanes](#) can thus have an infinite number of conformations by rotation around C-C single bonds. However, this rotation is not completely free due to repulsive interactions between the electron clouds of C-H bonds. This repulsive interaction is termed as torsional strain.

Conformational Isomers

Let us understand the fundamentals of conformation with the example of ethane. If we observe the ball and stick model of ethane and rotate one carbon atom keeping another carbon atom stationary about the C-C axis. We will observe that the rotations will result in an infinite number of spatial arrangements of hydrogen atoms attached to one carbon atom with respect to the hydrogen atoms attached to the

other carbon atom. These different arrangements are better known as **conformational isomers** or **conformers**.

Predominantly, these can be broadly classified into two different cases:

1. **Eclipse conformation**

Conformation in which hydrogen atoms are attached to two carbons stay nearest to each other as possible is known as eclipsed

2. **Staggered conformation**

Conformation in which hydrogen atoms attached to two carbons are as far as possible with respect to each other is known as staggered. The staggered conformation is thus relatively more stable in comparison to eclipse conformation as there are minimum repulsive forces, minimum energy due to many separations between the electron clouds of C-H bonds.