

Classification of Organic Compounds

Fundamentals

Why carbon?

- Can form single, double, triple bond.
- Can bond to itself, forming long chain (catenation) and rings (cyclic)
- Form tetrahedral when single bonded
- Stable compound due to bond strength and stability. ($C - C = 348 \text{kJmol}^{-1}$, $C - H = 412 \text{kJmol}^{-1}$)
- Can bond to a range of other elements.

Types of Organic Compounds

- Saturated (IHD = 0) / Unsaturated (IHD > 0)
- Aliphatics (No ring) / Arenes (Rings)
- Electrophile (Need electron) / Nucleophile (Have more electron)

Formulas

- Empirical formula: Simplest whole number ratio
- Molecular formula: Actual number of each element present
- Structural formula: Showing how the atoms are bonded to each other
 - Full: Show every bond and atom
 - Condensed: Omit bonds that can be assumed, group atoms together
- Skeletal formula: Omit Carbon and hydrogen atoms
- Stereochemical formula: Relative positions of atoms in three dimensions

Unknown parts of the molecule are noted as **R**

Degree of Unsaturation: IHD

$$\text{Index of Hydrogen Deficiency} = \frac{1}{2} \times (2C + 2 - x + N - H)$$

Or: Each double bond / ring count as 1, and triple bonds count as 2

Homologous Series

A group of organic compounds with the same and same number of functional groups.

- Differ from each other by a CH_2
- Can be represented by a general formula
- Have similar chemical properties
- Have physical properties that vary in regular manner as number of carbon increases.
 - Longer the carbon chain
 - Higher boiling point
 - Higher density
 - Higher viscosity

Functional Groups

Homologous series	Functional Group	Group Name
Alkane	/	Alkyl
Alkene	$C = C$	Alkenyl
Alkyne	$C \equiv C$	Alkynyl
Alcohol	OH	Hydroxyl
Ether	$C - O - C$	Ether
Aldehyde	CHO	Carbonyl
Ketone	$C - CO - C$	Carbonyl
Carboxylic Acid	$COOH$	Carboxyl
Halogenoalkane	Cl, Br, I	Halo
Amine	NH_2, NHR, NR_2	Amino
Ester	$COOC$	Ester
Nitrile	$C \equiv N$	Nitrile
Amide	$CO - NH_2$	Carboxamide

Arenes are compounds derived from benzene. (Functional group = Phenyl)

Primary, Secondary and Tertiary Compounds

These compounds has carbon atom attached to a functional group.

The carbon atom is

- Primary: connected to 1 carbon atom

- Secondary: connected to 2 carbon atoms
- Tertiary: connected to 3 carbon atoms

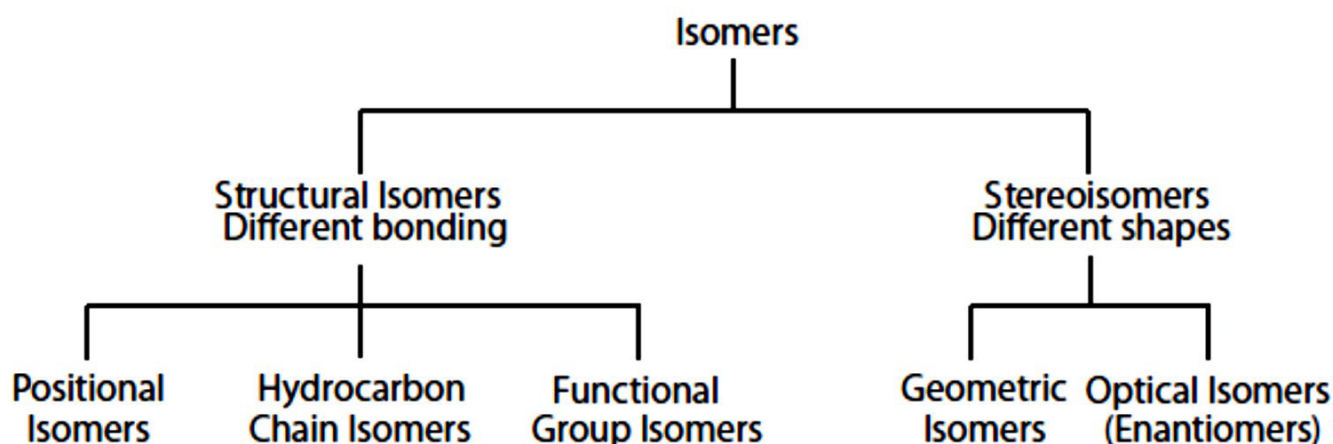
Same rule can be applied to nitrogen atoms.

Naming

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Isomers

Molecules with same molecular formula but different structures.



Structural Isomers

Molecules having the same molecular formula but the atoms are jointed in a different order.

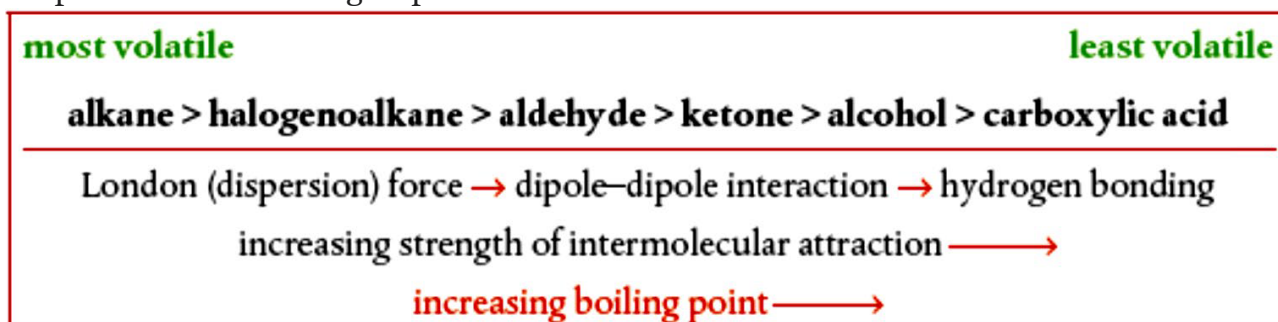
- **Positional Isomers**
 - Same hydrocarbon skeleton
 - Same number of functional group
 - Functional group is on different parts of skeleton
- **Hydrocarbon Chain Isomers**
 - Isomers have different hydrocarbon skeletons
 - Possible there's no functional groups
- **Functional Group Isomers**
 - Isomers having different types of functional groups
 - *Pairs of functional groups than can form isomers*

- Alcohol and Ether
- Alkene and Cycloalkane
- Aldehyde and Ketone
- Carboxylic acid and Ester

Different positional isomers and hydrocarbon chain isomers usually have similar chemical properties, while functional group isomers have very different properties.

Trends in Physical Properties

- Increase in boiling point with carbon number
- **Branched** hydrocarbon chain isomers has lower boiling points
 - Less contact with each other
 - Weaker intermolecular forces
- Properties of functional groups



Stereoisomers

Molecules with the same joining order of the atoms, but have a different arrangement of atoms in space and hence different three dimensional shapes.

- **Geometrical Isomers**
 - **Conformational Isomers**
 - Spontaneously interconvert by rotation, cannot be isolated separately.
 - **Configurational Isomers**

Permanent difference in geometry, cannot be interconverted, exist as separate compounds.

Include:

- Double bond (π bonds do not rotate because of p orbitals)

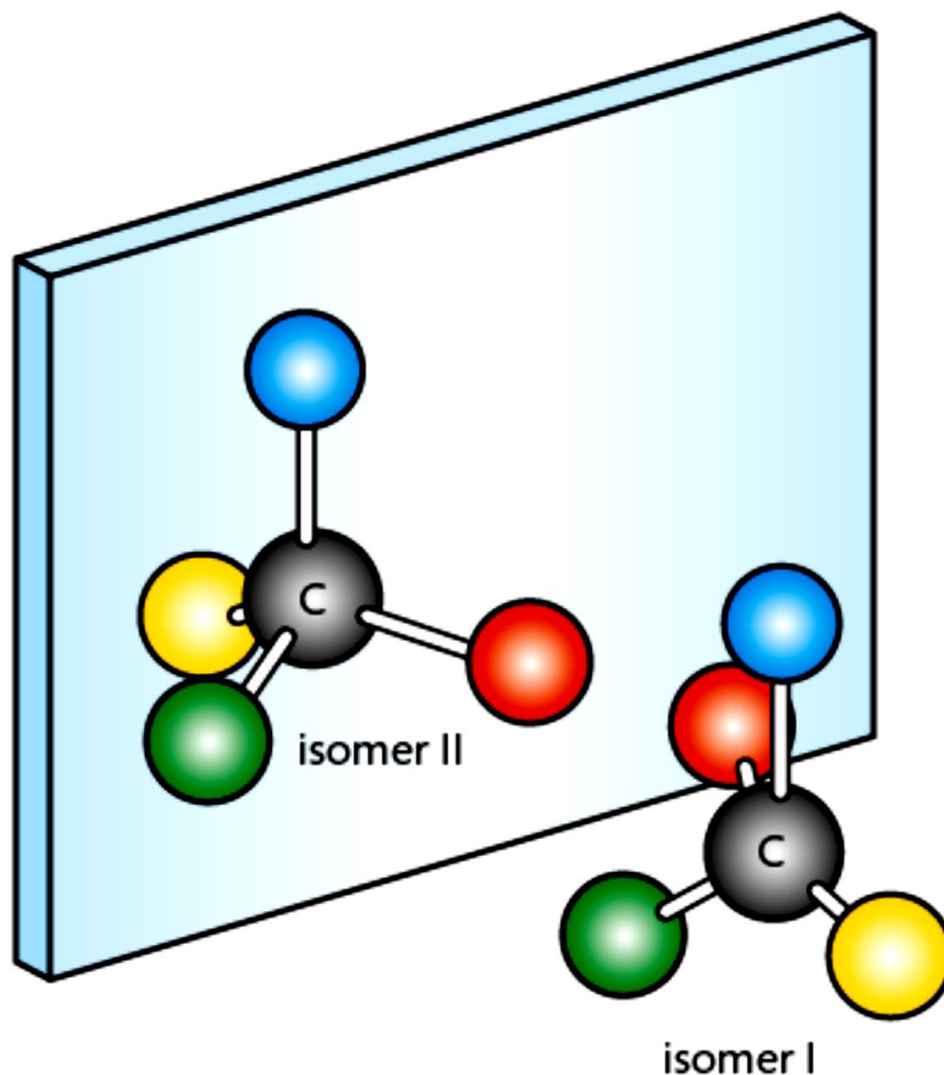
- Cyclic molecules (Different side to the reference plane)

There are two naming systems for these isomers:

- **Cis-Trans** isomers
 - Cis: Same group on same side of the double bond or ring.
 - Trans: Same group on different sides.
 - **Z/E** isomerism
 - Rule 1: Higher atomic number attached to the double bond carbon has higher priority.
 - Rule 2: If same atom, then same rule applied to next atom on the chain.
 - Note: $-OH$ and $-NH_2$ **DO NOT** attach to $C = C$ due to instability
 - Z: High priority on same side
 - E: High priority on opposite side
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- **Optical Isomers**

Has a **Chiral Carbon** (A carbon atom attached to four different atoms or groups).



The four groups, arranged tetrahedrally around the carbon atom with bond angles of 109.5° , can be arranged in two different three-dimensional configurations which are mirror images of each other.

- The property of not lining up is called **Non-Superimposable**
- **Enantiomers**: Two non-superimposable forms of optical isomers.
 - For each Chiral carbon, the arrangement is opposite for two Enantiomers
- **Racemic Mixture**: Mixture containing equal amounts of two **enantiomers**.
 - Optically Inactive
- **Diastereomers**: Optical isomers that has multiple chiral carbon but not all of them are opposite.
 - Not mirror images of each other
 - Have different configurations at *One, or more, but not all chiral centers*.

Properties of Enantiomers

- Optical Activity
 - Optical isomers can rotate the plane of polarization for plane-polarized light.
 - Could vary for different solution, concentrations of the solution, wavelength of light, sample path length.
 - **Optically Active**

Separate solutions of enantiomers, at the same concentration, rotate plane-polarized light in equal amounts but opposite directions.

 - Racemic mixture does not rotate the light - Optically inactive.
 - Natural molecules only produce one enantiomer.
- Reactivity with other chiral molecules
 - **Resolution:** Two enantiomers of a racemic mixture can be separated when reacting with another *chiral molecule*.