INTRODUCTION TO ORGANIC CHEMISTRY

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Introduction to Organic Chemistry

Catenation: bonding of atoms of the same element a chain or ring.

Catenation occurs most readily with carbon, which forms covalent bonds with other carbon atoms to form chains and rings. This is the reason for the presence of the vast number of organic compounds in nature.

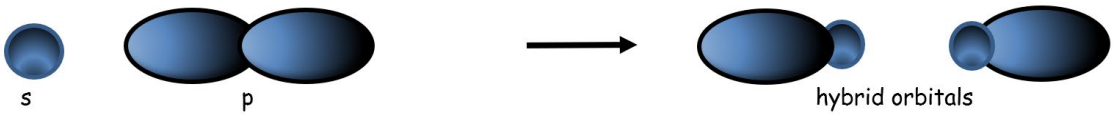
Carbon Bonding

Carbon atom
Electron arrangement: 2:4
$1s^2s^2 2p^2$

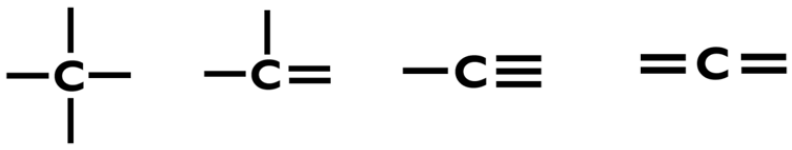
C-C covalent bond

Carbon atoms link together (catenate) to form stable chains and rings containing strong single, double and triple bonds

Hybridisation of atomic orbitals



Note: the number of hybrid atomic orbitals equals the number of atomic orbitals that 'fuse'. Three 'p' orbitals and one 's' orbital form four sp^3 hybrid orbitals.



sp^3 **sp^2** **sp** **sp^2** **sp^2**

Carbon atoms can form:

- 4 single covalent bonds (sp^3 hybrid orbitals)
- 2 single and a double covalent bond (sp^2 hybrid orbitals)
- 1 single and a triple covalent bond (sp hybrid orbitals)
- 2 double covalent bonds (sp^2 hybrid orbitals)

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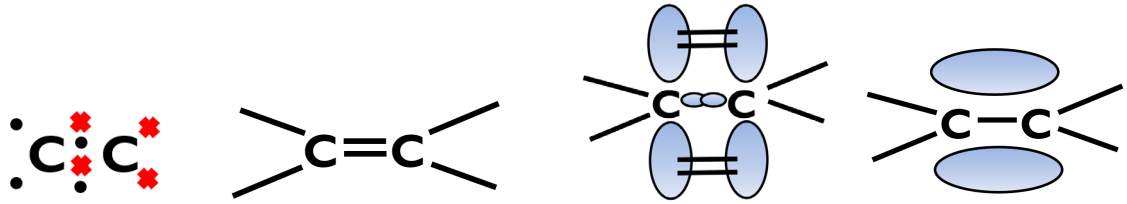
Carbon-Carbon Double Bond

Carbon-Carbon double bonds comprise a sigma (σ) and a pi (π)

Sigma (σ): end-to-end overlap of sp^2 orbitals. Electrons are located between the nuclei of the bonding atoms.

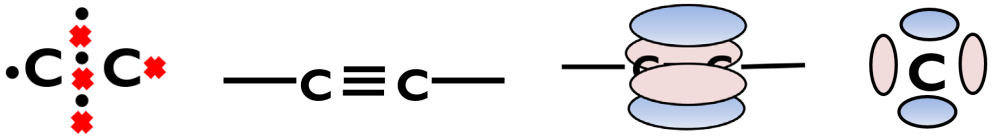


Pi (π): side-by-side overlap of p orbitals. Electrons are located above and below the plane of

Carbon-Carbon Triple Bond

Carbon-Carbon triple bonds comprise a sigma (σ) and two pi (π) bonds.

Sigma (s): end-to-end overlap of sp orbitals. Electrons are located between the nuclei of the bonding atoms.



Pi (π): side-by-side overlap of p orbitals. The two sets of overlapping p orbitals are at right angles to each other.

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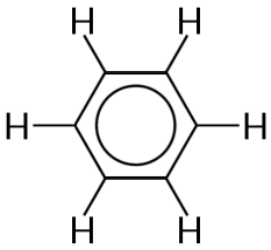
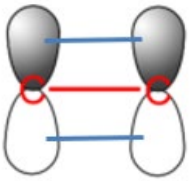
Bonding in Benzene

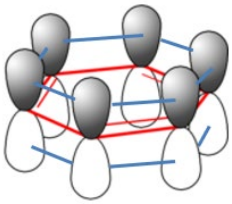
The circle represents the delocalised electrons.

The 6 π electrons are delocalised in a ring structure above and below the plane of the molecule.



C-H sigma (σ) bond





sp^2

sigma (σ) bond (red) overlap of sp^2 orbitals

Benzene is a planar regular hexagon, with bond angles of 120°.

Carbon-carbon bond length is in between that of C-C and C=C.

pi (π) bond (blue) sideways overlap of p

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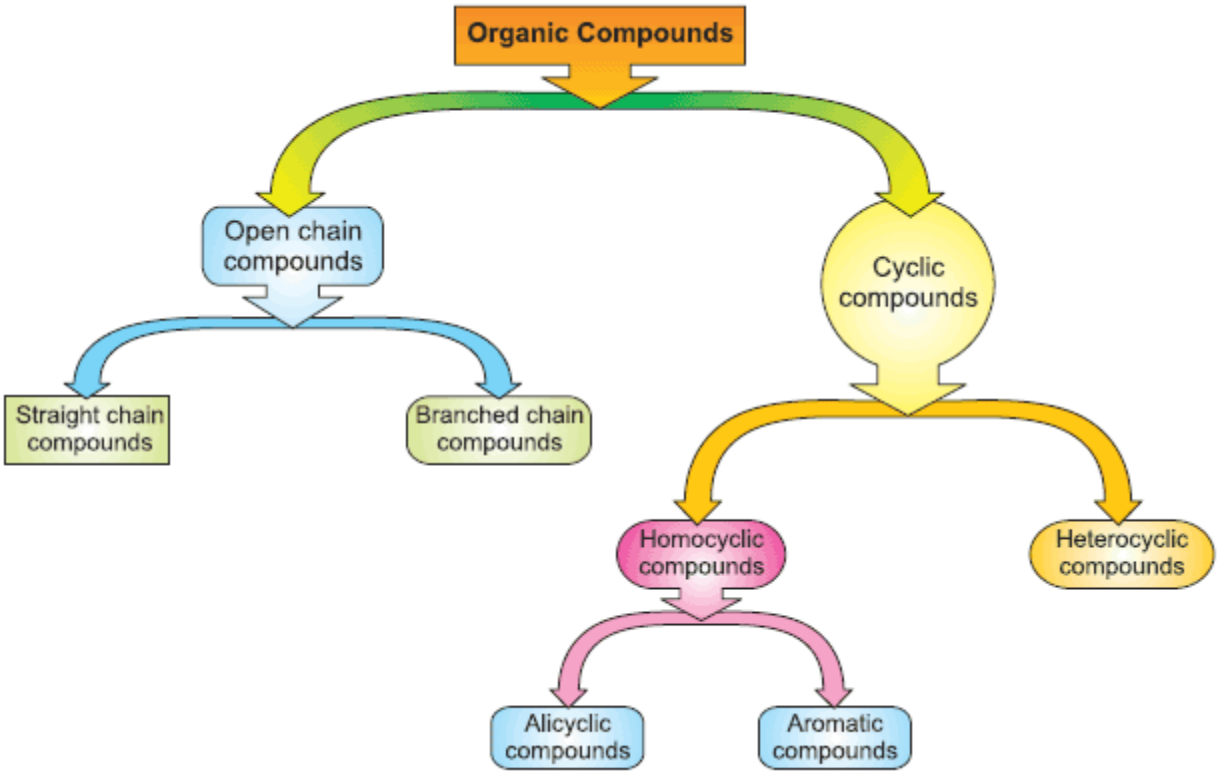
Classifying Organic Compounds



Open Chain Compounds

- Straight carbon chains
- Branched carbon chains

Cyclic Compounds

- Homocyclic compound: rings made from only carbon atoms
- Heterocyclic compounds: rings made from one or two atoms other than carbon

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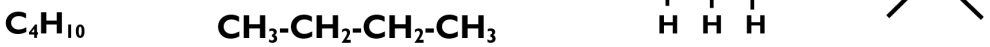
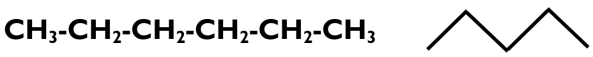
Aliphatic Compounds

Chemists use a range of "diagrammatic" shorthand when writing organic structures.

molecular formula **structural formula** **skeletal formula**



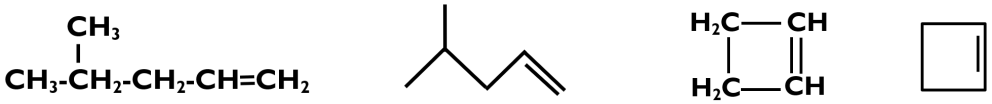
butane propane (C_3H_8)



linear chains

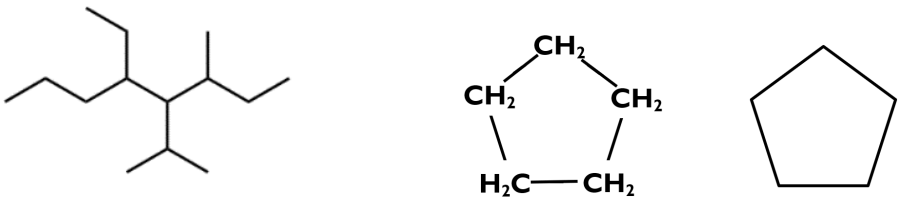
hexane

unsaturated



4-methylpent-1-ene cyclobutene

branched chains **rings**



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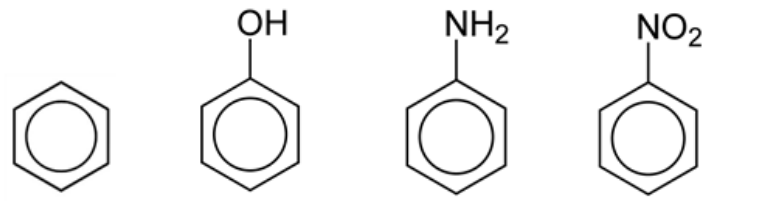
Aromatic Compounds

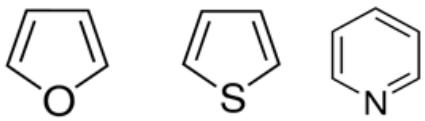
Aromatic compounds, also known as arenes or aromatics, are compounds that contain conjugated planar ring systems with delocalized pi electron clouds instead of discrete alternating single and double bonds.



benzene (C_6H_6) | phenol (C_6H_5OH) | aniline ($C_6H_5NH_2$) | nitrobenzene ($C_6H_5NO_2$)

Heterocyclic Compounds

Heterocyclic compounds, are cyclic compounds with the ring containing carbon and other element, the component being oxygen, nitrogen and sulfur.



furan (C_4H_4O) | thiophene (C_4H_4S) | pyridine (C_5H_5N)

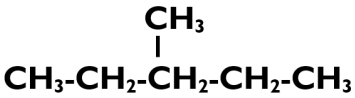
Isomerism

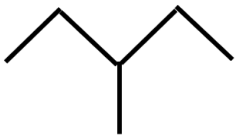
Structural Isomers: molecules that have the same molecular formula but with the atoms connected in a different order.

Structural Isomers of C_6H_{14}

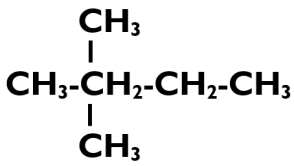
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

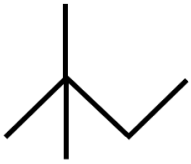
n-hexane



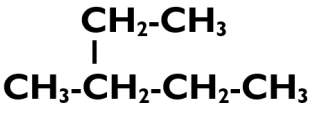


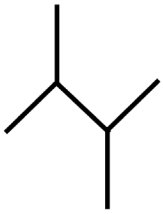
3-methylbutane





2,2-dimethylbutane





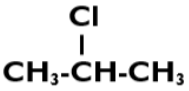
2-ethylbutane

Structural isomers often exhibit different physical and chemical properties. Branched chain isomers have lower densities, melting and boiling temperatures than the equivalent linear isomer.

Isomerism

Positional Isomers: have the same carbon skeleton and the same functional groups but differ from each other in the location of the functional groups on or in the carbon chain.

Example: C_3H_5Cl



2-chloropropane

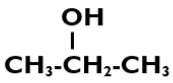
$CH_3\text{-}CH_2\text{-}CH_2\text{-}Cl$ 1=chloropropane

Functional Group Isomers: same molecular formula (that is, the same number of atoms of the same elements), but the atoms are connected in different ways so that the groupings are dissimilar.

Example: C_3H_6O

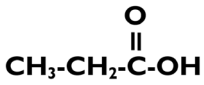
propan-1-ol (primary alcohol) $CH_3\text{-}CH_2\text{-}CH_2\text{-}OH$

propan-2-ol (secondary alcohol)

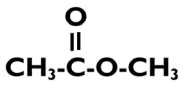


methoxyethane (ether) $CH_3\text{-}O\text{-}CH_2\text{-}CH_2$

Example: $C_3H_6O_2$



propanoic acid (carboxylic acid)

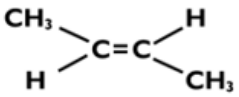


methylethanoate (ester)

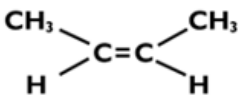
Stereoisomers

Stereosiomers - two main types - geometric **isomers** and optical **isomers**.

Geometric (configuration) Isomers:



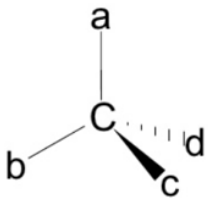
trans-but-2-ene

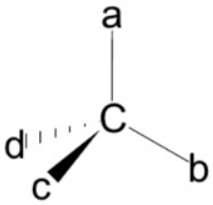


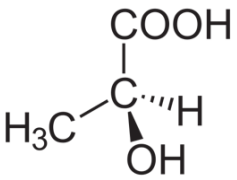
cis-but-2-ene

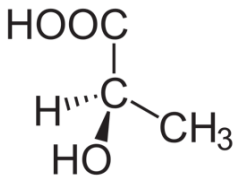
Optical Isomers: compounds which contain the same number and kinds of atoms, and bonds (i.e., the connectivity between atoms is the same), and different spatial arrangements of the atoms, but which have non-superimposable mirror images.

Optical isomerism exist as two isomers - **enantiomers**.





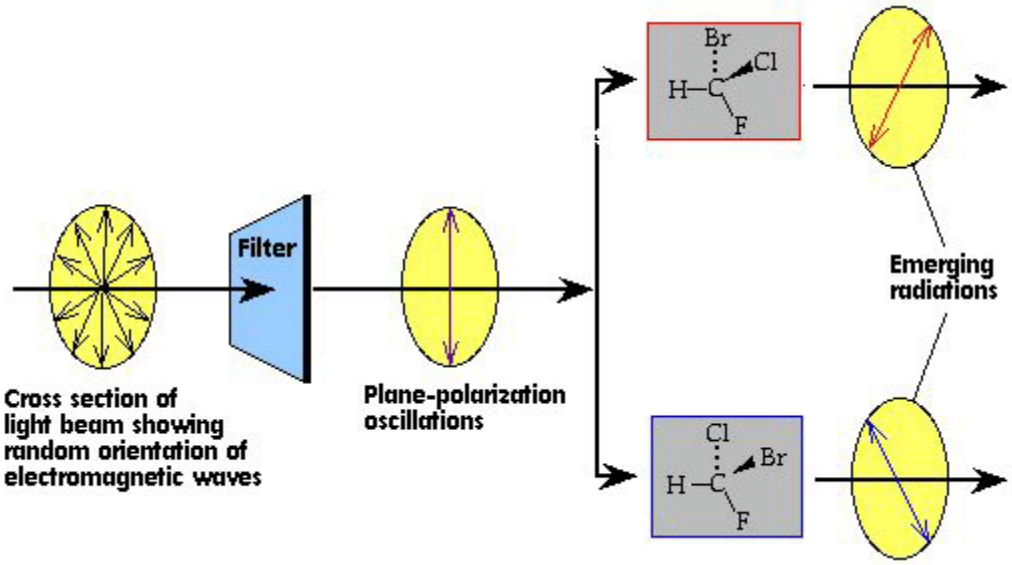




Chiral carbons are bonded to four different substituents.

Optical isomers can rotate the plane of plane-polarised light.

Stereoisomers



Properties of optical isomers:

They rotate plane polarised light.

One isomer rotates it in one direction and the other in the opposite direction.

An equal mixture of the 2 isomers will not rotate plane polarised light as each isomer cancels the other out. This mixture is known as a **racemic** mixture.