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# Chapter 15 (AS-Level)

## Introduction to Organic chemistry

***Organic chemistry is the study of compounds containing hydrogen and carbon and of compounds containing other elements in addition to carbon and hydrogen.***

Why are there many different carbon compounds? This is mainly due to:

- Carbon readily bonding to itself and to most other elements including metals (organometallic)
- Carbon can bond in a variety of ways giving rise to chains, rings and cages.

Compounds that only contain carbon and hydrogen are called hydrocarbons. They are classified as aliphatic or aromatic.

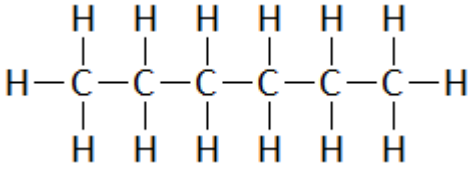
Aromatic compounds contain one or more arene rings. They have distinctive, usually pleasant smells. All the other organic compounds are aliphatic.

For example, all alkanes and alkenes are aliphatic and benzene is an aromatic compound.

## Types of formulae

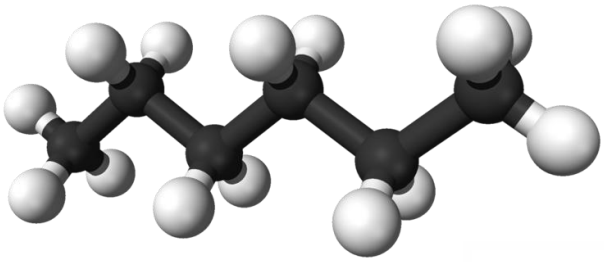
There are some forms of formulae to remember:

- Molecular formula: it simply shows the number of atoms of each element present in the molecule. For example, hexane is $C_6H_{14}$
- General formula: it may be written for a series of compounds. For example, for alkanes, it is $C_nH_{2n+2}$, where n is the number of carbon atoms
- Structural formula: it shows how the atoms are joined together in a molecule. For example, in hexane, it is $CH_3CH_2CH_2CH_2CH_2CH_3$
- Displayed formula: shows all the bonds and all the atoms For example hexane,



- Skeletal formula: shows all the bonds and all the atoms. Again, for example, hexane,

- Three dimensional formula: gives you the best representation of a molecule.



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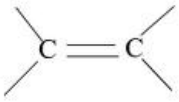
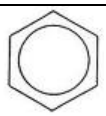
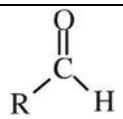
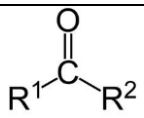
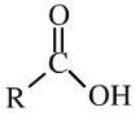
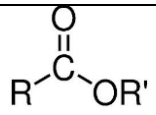
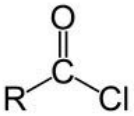
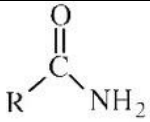
## Functional groups

Each group of atoms that becomes attached to carbon has its own characteristic set of reactions. Each functional group gives rise to a homologous series which are molecules with the same functional group but with different lengths of carbon chains.

For example, the functional group (-OH), gives rise to the homologous series of alcohols. They all have similar chemical properties. A general formula may be written for the aliphatic alcohols which is $C_NH_{2N+1}OH$.

Some examples of functional groups are:

| Class of functional groups | Structure of functional groups | Name of example | Structural formula of example |
|---|---|---|---|
| Alkenes |  | Ethene | $CH_2=CH_2$ |
| Arenes |  | Benzene | |
| Halogenoalkanes | -X, where X= F, Cl, Br, I | Chloromethane | $CH_2Cl$ |
| Alcohols and phenols | -OH | Methanol, phenol | $CH_3OH$, $C_6H_5OH$ |
| Aldehydes |  | Ethanal | $CH_3CHO$ |
| Ketones |  | Propanone | $CH_3COCH_3$ |
| Carboxylic acids |  | Ethanoic acid | $CH_3COOH$ |
| Esters |  | Ethyl ethanoate | $CH_3COOC_2H_5$ |
| Acyl chlorides |  | Ethanoyl chloride | $CH_3COCl$ |
| Amines | -NH2 | Methylamine | $CH_3NH_2$ |
| Amides |  | Ethanamide | $CH_3CONH_3$ |
| Nitriles | -C≡N | Ethanenitrile | $CH_3CN$ |

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## Naming organic compounds

There are two way of naming organic compounds:

- Common names
- Systematic names (IUPAC names)

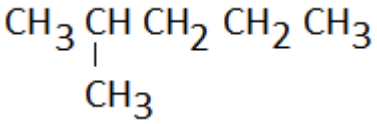
| Prefix | Stem | Suffix |
|---|---|---|
| Side chain, with numbers | Derived from the longest carbon chain of alkane. E.g. Methane, ethane, etc. | Indicates functional groups. E.g. Ane, ene, al, ol, one, oic acid. |

Basic rules for naming hydrocarbons:

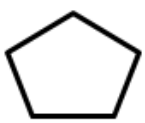
1. The number of carbon atoms in the longest unbranching chain provides the stem of the name. They are named by adding –ane to the stem.

| Molecular formula | # of C atoms in longest chain | Stem | Name |
|---|---|---|---|
| $CH_4$ | 1 | Meth- | Methane |
| $C_2H_6$ | 2 | Eth- | Ethane |
| $C_3H_8$ | 3 | Prop- | Propane |
| $C_4H_{10}$ | 4 | But- | Butane |
| $C_5H_{12}$ | 5 | Pent- | Pentane |
| $C_6H_{14}$ | 6 | Hex- | Hexane |

2. Branched alkanes are named the same way in (1). The name is given to the longest unbranching carbon chain. It is then prefixed by the names of the shorter side-chains. The stem names are used with the suffix –yl. For example, CH3- is methyl group (alkyl group). The position of the alkyl group is indicated by the number of the carbon atom that the alkyl group is on. Numbering starts from the end that produces the lowest possible numbers for the side-chains.
   For example, the following is 2, methylpentane.



3. Each side chain must be included in the name.
   - If there are identical side-chains, the name is prefixed with di-, tri, tetra-, etc. For example, 2,2,3-trimethyl- indicates that there are three methyl groups, two on carbon 2 and one on carbon 3.
   - If there are different alkyl groups, they are placed in alphabetical order. For example, 3-ethyl-2-methylpentane.
4. Compounds that have a ring of carbon atoms, the stem is prefixed by cyclo-. For example, cyclopentane is:



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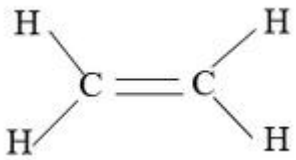
5. In alkanes where there is an alkene or arene group:
   Alkene: ethene



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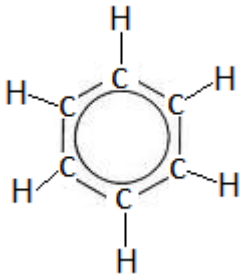
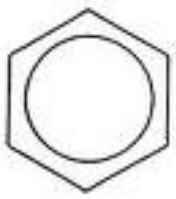
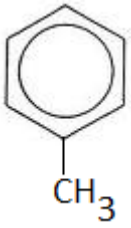
   Arene: benzene

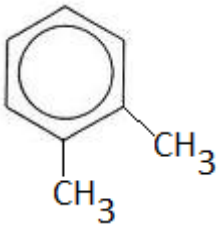


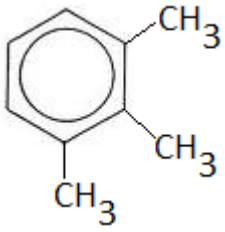


   Displayed formula  Skeletal formula

   - The hydrocarbons with one double bond are called alkenes. The position of the double bond is indicated by the lower number of the two carbon atoms involved. This number is placed between the stem and the –ene. For example, $CH_3CH=CHCH_3$ is but-2-ene.
   - The simplest arene is benzene. When one alkyl group is attached to a benzene ring, a number is not needed because all the carbon atoms are equivalent. Two or more groups will require a number. For example:

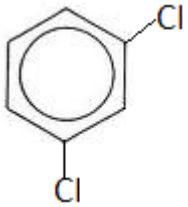






   Methylbenzene  1,2-dimethylbenzene  1,2,3-trimethylbenzene

6. In halogeno compounds, the name is the same as alkyl- substituted alkenes or arenes.
   $CH_3CH_2CHBrCH_3$



   2-Bromobutane  1,3-dichlorobenzene

7. In aliphatic alcohols and ketones are named in a similar way to alkenes.

| | |
|---|---|
| $CH_3CH_2CH_2OH$ | $CH_3CH_2COCH_3CH_3$ |
| Propan-1-ol | Pentan-3-one |

   In aliphatic aldehydes and carboxylic acids, no numbers are needed.

| | |
|---|---|
| $CH_3CH_2CHO$ | $CH_3CH_2COOH$ |
| Propanal | Propanoic acid |

8. In amines, use alkyl or aryl prefix followed by the word amine. For example, $CH_3CH_2NH_2$ is ethylamine.

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## Organizing organic reactions

There are several organic reactions, which include:

- Acid-base reactions, for example, Ethanoic acid reacts with sodium hydroxide to form sodium ethanoate and water:

$$CH_3COOH\ (aq) + NaOH\ (aq) \rightarrow CH_3COONa\ (aq) + H_2O\ (l)$$

- Redox reactions, for example, between ethanol and oxygen:

$$CH_3CH_2OH\ (aq) + O_2\ (g) \rightarrow CH_3COOH\ (aq) + H_2O\ (l)$$

- Substitution reactions, which involves replacing an atom by another atom. For example, the bromine atom in bromoethane is substituted by the –OH group to form ethanol when it is warmed with sodium hydroxide:

$$CH_3CH_2Br\ (l) + OH^-\ (aq) \rightarrow CH_3CH_2OH\ (aq) + Br^-\ (aq)$$

- Addition reactions, which involve 2 molecules combining to make only one new molecule. For example, if ethene and steam is passed over a hot phosphoric acid catalyst, ethanol is produced:

$$CH_2{=}CH_2\ (g) + H_2O\ (g) \rightarrow CH_3CH_2OH\ (g)$$

- Elimination reactions, which involve the removal of a molecule from a larger one. For example, is ethanol is passed over a hot catalyst of pumice, a water molecule is eliminated:

$$CH_3CH_2OH\ (g) \rightarrow CH_2{=}CH_2\ (g) + H_2O\ (g)$$

- Hydrolysis reactions involve breaking covalent bonds by the reaction with water. For example, when bromoethane is mixed with water, ethanol is formed along with hydrogen bromide:

$$CH_3CH_2Br\ (l) + H_2O\ (l) \rightarrow CH_3CH_2OH\ (aq) + HBr\ (aq)$$

## Reaction mechanisms

A balanced chemical equation includes no information about the reaction pathway. The reaction pathway includes details of the intermediate chemical species which exist between the reactants and products. The activation energy is the energy needed to form these transient species. Catalysts increase the reaction rate by providing an alternative pathway for the reaction with lower activation energy.

If a reaction pathway with lower activation energy is found, more molecules will have sufficient energy to react. Catalysts take part in the reaction mechanism but remain unchanged at the end of the reaction so they don't appear in the chemical equation.

### Breaking bonds in different ways

A covalent bond consists of a pair of electrons between 2 nuclei in which they are attracted to the nuclei. This binds the 2 nuclei together. Covalent bonds can be broken in many ways.

For example, if HCl is broken into H and Cl atoms, each atom takes one electron from the covalent bond. Atoms with unpaired electrons are called free radicals. When a covalent bond is broken to form 2 free radicals, the process is called homolytic fission. The energy for this process is usually provided by UV light or high temperature.

Unpaired electrons are represented by a dot.

$$HCl \rightarrow H^{\cdot}(g) + Cl^{\cdot}(g)$$

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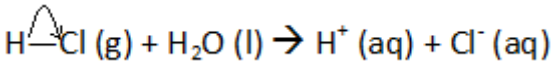
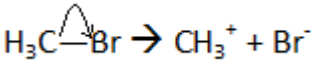
Alternatively, a covalent bond may be broken so that one element takes both covalent bond electrons. For example, HCl would form hydrogen and chloride ions:

$$HCl \rightarrow H^+ + Cl^-$$

The more electronegative element takes both the electrons. When a covalent bond is broken to form 2 oppositely charged ions, the process is called heterolytic fission. The bond in the HCl breaks heterolyticly when the gas dissolves in water to form hydrochloric acid. The movement of the two electrons is shown by a curly arrow. For example, when HCl dissolves in water:



Another example is the heterolytic fission of bromomethane:



Positively charged ions that contain carbon are called carbocations. A negatively charged ions containing carbon is called a carbanion.

Free radicals, carbocations and carbanions are all highly reactive species. They react with molecules, causing covalent bonds to break and new covalent bonds to form.

Carbocations and carbanion are electrophiles and nucleophiles respectively.

***An electrophile is an electron-loving (and an electron-poor) species and is a proton acceptor and is attracted to electron-rich molecules, leading to the formation of a new covalent bond between the electrophile and thee molecule.***

***A nucleophile (nucleus-lover) is an electron-pair donor which is attracted to an atom with a partial positive charge, leading to the formation of a new covalent bond between the nucleophile and the molecule under attack.***

## Isomerism

Isomers have the same molecular formula but a different structural formula. Isomerism is due to a number of reasons, which include the ability of carbon being able to bond to itself and to most other carbon atoms in the periodic table.

### Structural isomerism

Structural isomerism describes the situation where chemicals of the same formula behave differently because the structures are the same. For example, the atoms of butane can be put together in 2 ways, which is it has 2 isomers.

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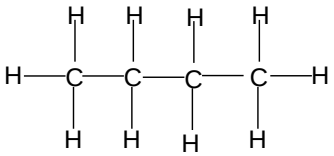
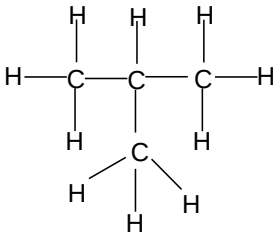


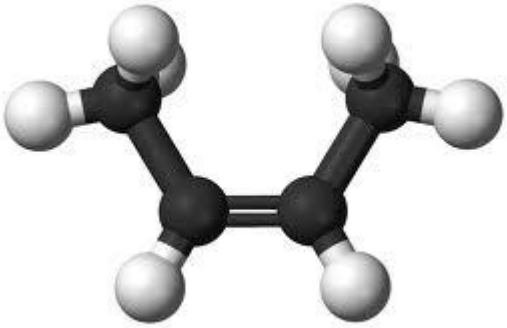


## Stereoisomerism

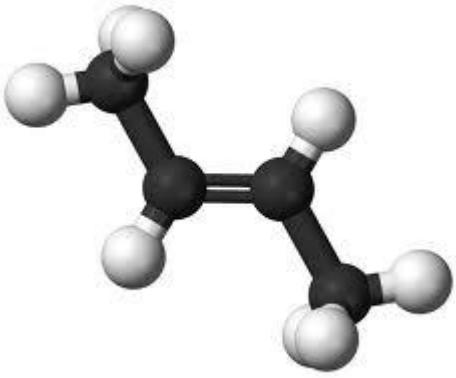
In stereoisomerism, the same atoms are joined to each other in different spatial arrangements. Geometric and optical isomerism are two types of this stereoisomerism.

### Geometric (or cis-trans) isomerism

The atoms on either side of a carbon-carbon single bond can rotate freely, but the atoms around a carbon=carbon double bond cannot. For example, but-2ene, $CH_3CH=CHCH_3$ has 2 cis-trans isomers.



Cis-but-2-ene



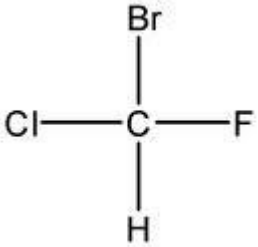
Trans-but-2-ene

## Optical isomerism

The simplest form of optical isomerism occurs when a carbon atom is joined to four different groups. The groups can be arranged in 2 different ways and the 2 isomers formed are mirror images of each other, which cannot be superimposed. These two optical isomers are also chiral molecules, which are molecules which are mirror images and cannot be superimposed.

Optical isomerism is sometimes referred to as chirality. The carbon atom in the centre which carries the four different groups is called the chiral centre.

Optical isomers, like other isomers, have the same molecular formula. As stereoisomers, they have the same atoms and the same bonds between the atoms. However, here, the bonds are arranged differently in space. For example, the molecule CHBrClF provides a good example of optical isomerism.



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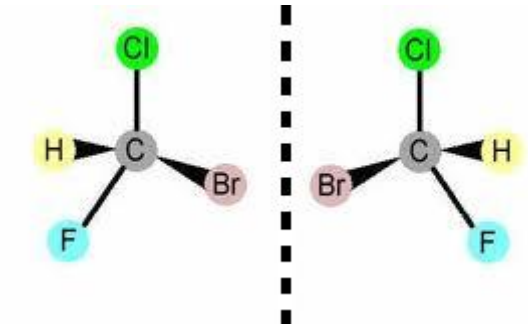
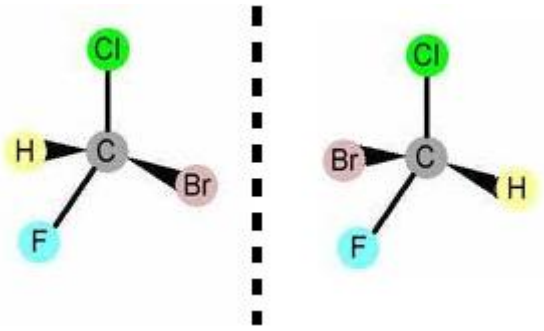
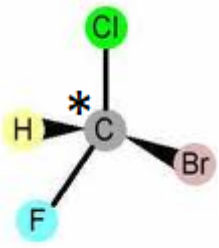
To display the optical isomers, we need to use three-dimensional formula, in which the dotted line in the middle shows a mirror plane:




If the right hand molecule is rotated around the C-Cl bond, it produces:




The atoms Cl, C and F are in the same spatial position, but the H and Br are interchanged. If the two isomers are placed over each other (superimposed) they don't match. We say that they are non-superimposable. The key feature of a chiral centre in an organic molecule is that it has 4 different groups attached to it. The chiral centre in this molecule (Chloro-fluoro-bromo-methane) is labeled with a small star.




***END OF LESSON***

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