

14 Organic: Basic Concepts

Basic definitions to know

Hydrocarbon is a compound consisting of hydrogen and carbon **only**

Saturated: Contain single carbon-carbon bonds only

Unsaturated : Contains a C=C double bond

Molecular formula: The formula which shows the actual **number of each type of atom**

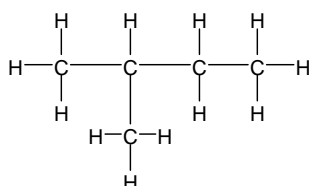
Empirical formula: shows the simplest whole number ratio of atoms of each element in the compound

General formula: algebraic formula for a homologous series e.g. C_nH_{2n}

Structural formula shows the minimal detail that shows the arrangement of atoms in a molecule, eg for butane: $CH_3CH_2CH_2CH_3$ or $CH_3(CH_2)_2CH_3$,

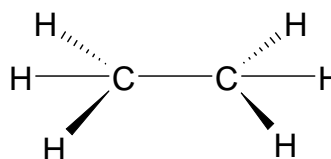
Displayed formula: show all the covalent bonds and atoms present in a molecule

Drawing Displayed formulae

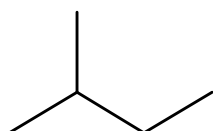


When drawing organic compounds add the hydrogen atoms so that each carbon has 4 bonds

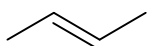
Remember that the shape around the carbon atom in saturated hydrocarbons is tetrahedral and the bond angle is 109.5°



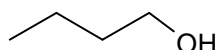
Skeletal formula shows the simplified organic formula, shown by removing hydrogen atoms from alkyl chains, leaving just a carbon skeleton and associated functional Groups.



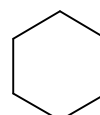
2-methylbutane



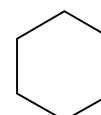
But-2-ene



Butan-1-ol



cyclohexane



cyclohexene

Functional group is an atom or group of atoms which when present in different molecules causes them to have similar chemical properties

Homologous series are families of organic compounds with the **same functional group** and **same general formula**.

- They show a gradual change in physical properties (e.g. boiling point).
- Each member differs by CH_2 from the last.
- same chemical properties.

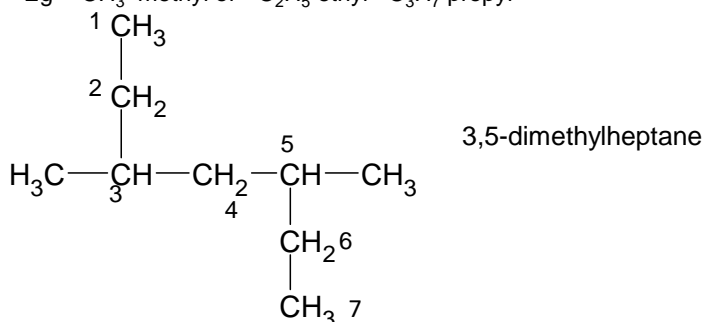
homologous series	functional group	prefix / suffix (* = usual use)	example
Alkane		-ane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ Butane
Alkenes		suffix -ene	propene
Alcohols		suffix* -ol prefix hydroxy-	Propan-1-ol
Halogenoalkanes		prefix chloro- bromo- iodo-	1-chloropropane
Aldehydes		suffix -al prefix formyl-	ethanal
Ketones		suffix* -one prefix oxo-	Propanone
carboxylic acids		suffix -oic acid	Ethanoic acid
Esters		-yl -oate	methylethanoate

homologous series	functional group	prefix / suffix (* = usual use)	example
nitriles		suffix -nitrile prefix cyano-	 Propanenitrile
amines		suffix* -amine prefix amino-	 Propylamine Or propan-1-amine
Acyl chloride		-oyl chloride	 ethanoylchloride
Amide		-amide	 ethanamide

General rules for naming carbon chains

- Count the longest carbon chain and name appropriately
- Find any branched chains and count how many carbons they contain
- Add the appropriate prefix for each branch chain

Eg -CH₃ methyl or -C₂H₅ ethyl -C₃H₇ propyl



code	no of carbons
meth	1
eth	2
prop	3
but	4
pent	5
hex	6
hept	7
oct	8
non	9
dec	10

Basic rules for naming functional groups

The functional group is named by a prefix or suffix. e.g. **bromoethane**, **ethanol**, **propene**

- When using a suffix, add in the following way :

If the suffix starts with a vowel- remove the -e from the stem alkane name
e.g. Propan-1-ol, butan-1-amine, ethanoic acid, ethanoylchloride, butanamide

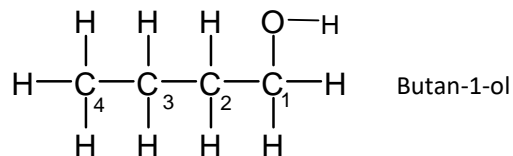
If the suffix starts with a consonant or there are two or more of a functional group meaning di, or tri needs to be used then **do not remove the the -e** from the stem alkane name
e.g. Propanenitrile, ethane-1,2-diol, propanedioic acid, propane-1,2,3-triol, Pentane-2,4-dione.

When compounds contain more than one functional group, the order of precedence determines which groups are named with prefix or suffix forms. The highest precedence group takes the suffix, with all others taking the prefix form. However, double and triple C-C bonds only take suffix form.

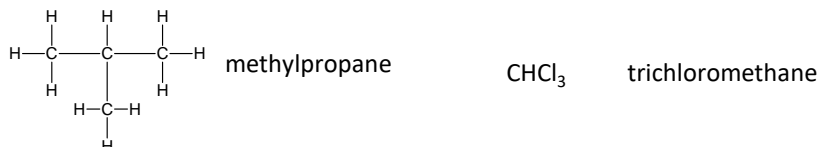
Order of priority highest first:

Carboxylic acids > carboxylic acid derivative > nitriles > aldehydes > ketones > alcohols > amines > alkenes > halogenoalkanes

• The position of the functional group on the carbon chain is given by a number – counting from the end of the molecule that gives the functional group the lowest number. For aldehydes, carboxylic acids & nitriles, the functional group is always on carbon 1.



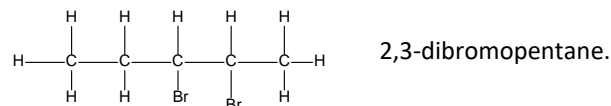
• We only include numbers, however, if they are needed to avoid ambiguity.



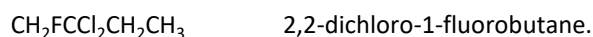
• The functional groups take precedence over branched chains in giving the lowest number

3-methylbut-1-ene is correct and not 2-methylbut-3-ene

• Where there are two or more of the same groups, **di-**, **tri-**, **tetra-**, **penta-** or **hexa-** are used. Note the point made above about the addition of 'e' to the stem



• Words are separated by numbers with dashes



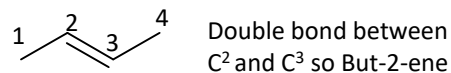
• numbers are separated by commas



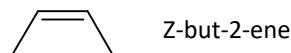
• If there is more than one functional group or side chain, the groups are listed in alphabetical order (ignoring any *di*, *tri*).

Alkenes

The double bond will be between two carbons. Use the lower number of the two to show the position of the double bond



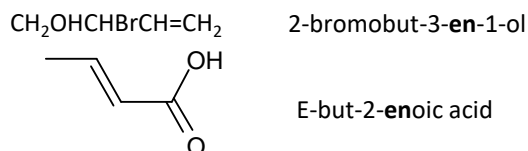
The name for alkenes may include E or Z at start to show the type of stereoisomer



If more than one double bond is present then suffix ends **diene** or **triene**. The stem ends in **a**

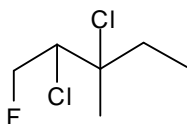
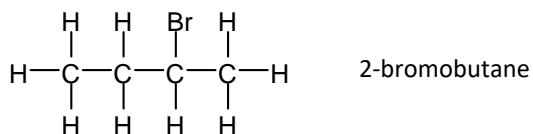


The suffix **-en** for alkenes can go in front of other suffixes. The alcohol and carboxylic acid groups have higher priority than the alkene group so take precedence with numbering

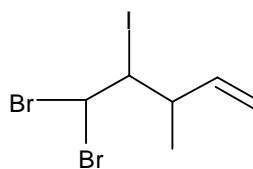


Halogenoalkanes

Class the halogen as a substituent on the C chain and use the suffix **-fluoro**, **-chloro**, **-bromo**, or **-iodo**. (Give the position number if necessary)



2,3-dichloro-1-fluoro-3-methylhexane



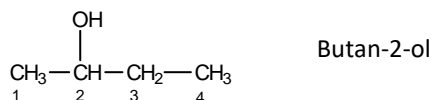
5,5-dibromo-4-iodo-3-methylpent-1-ene

Multiple functional group and side chains are listed in alphabetical order (ignoring any *di*, *tri*).

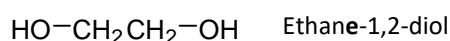
The alkene group has higher priority than the halogenoalkane group so it takes the lowest number on the carbon chain

Alcohols

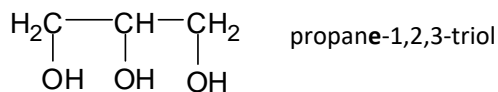
These have the ending **-ol** and if necessary the position number for the OH group is added between the name stem and the **-ol**



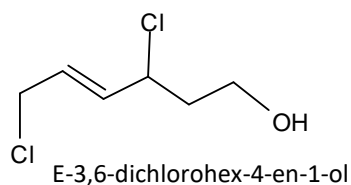
If there are two or more -OH groups then *di*, *tri* are used.



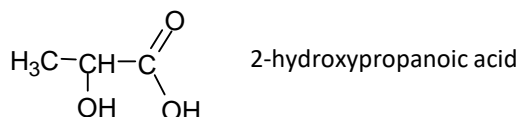
Add the **'e'** on to the stem name though.



The OH group has a higher priority than the halogenoalkane group and alkene so takes precedence in numbering. The OH is on carbon 1



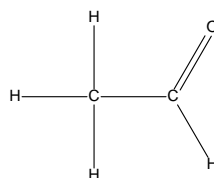
If the compound has an -OH group in addition to another functional group with a higher priority. The priority group gets the suffix ending and the OH can be named with the prefix **hydroxy-**:



Aldehydes

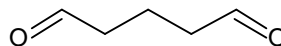
An aldehyde's name ends in **-al**

It always has the C=O bond on the first carbon of the chain so it does not need an extra number. It is by default number one on the chain.



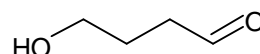
Ethanal

If two aldehyde groups then **di** is put before **-al** and an **e** is added to the stem.



pentanedial

Aldehydes have a higher priority than alcohol so the **-OH** group uses the hydroxy prefix.



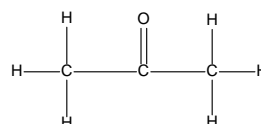
4-hydroxybutanal

Ketones

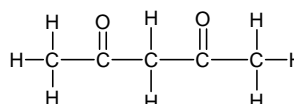
Ketones end in **-one**

When ketones have 5C's or more in a chain then it needs a number to show the position of the double bond. E.g. pentan-2-one

If two ketone groups then **di** is put before **-one** and an **e** is added to the stem.



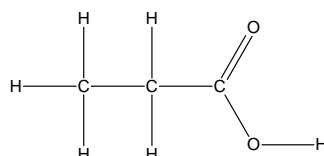
Propanone



Pentane-2,4-dione

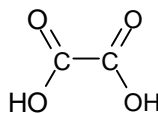
Carboxylic acids

These have the ending **-oic acid** but no number is necessary for the acid group as it must always be at the end of the chain. The numbering always starts from the carboxylic acid end.



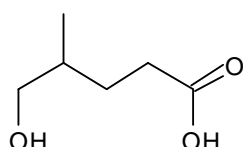
Propanoic acid

If there are carboxylic acid groups on both ends of the chain then it is called a -dioic acid



Ethanedioic acid

Note the **e** in this name



5-hydroxy-4-methylpentanoic acid

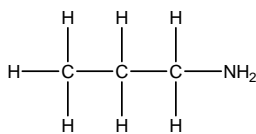
Amines

These end in **-amine**.

There is, however, rather confusingly two ways of using this suffix.

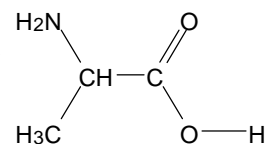
The exam board tend to use the common version where the name stem ends in **-yl** propylamine.

The IUPAC version of the same chemical is propan-1-amine. (This is used in the same way as naming alcohols)



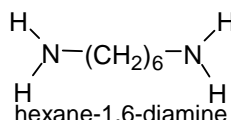
propylamine
Or propan-1-amine

If there is another priority functional group as well as the amine group then the prefix amino is used.



2-aminopropanoic acid.

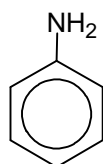
If there are two amine groups then name as following



hexane-1,6-diamine

It could also be named
1,6-diaminohexane

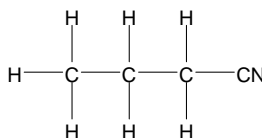
If amine groups are attached to a benzene ring then name as following



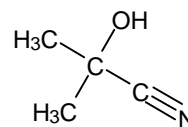
phenylamine

Nitriles

These end in **-nitrile**, but the C of the CN group counts as the first carbon of the chain. Note the stem of the name is different: butanenitrile and not butannitrile.



butanenitrile



2-hydroxy-2-methylpropanenitrile

Carboxylic acid derivatives

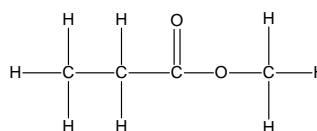
Esters

Esters have two parts to their names

The bit ending in **-yl** comes from the alcohol that has formed it and is next to the single bonded oxygen.

The bit ending in **-anoate** comes from the carboxylic acid.

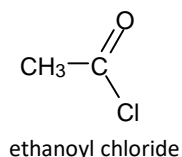
(This is the chain including the C=O bond)



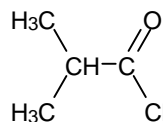
methylpropanoate

Acyl Chlorides

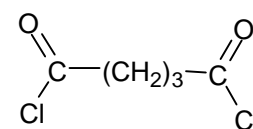
add **-oyl chloride** to the stem name



ethanoyl chloride



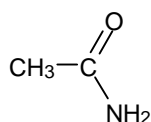
2-methylpropanoyl chloride



Pentanedioyl dichloride

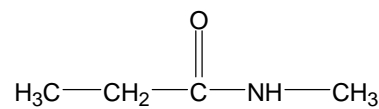
Amides

Add **-amide** to the stem name

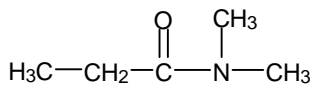


ethanamide

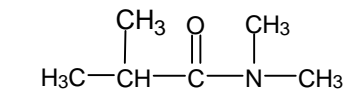
Secondary and tertiary amides are named differently to show the two (or three) carbon chains. The smaller alkyl group is preceded by an -N which plays the same role as a number in positioning a side alkyl chain



N-methylpropanamide



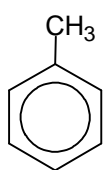
N,N-dimethylpropanamide



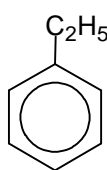
N,N,2-trimethylpropanamide

Naming aromatic molecules

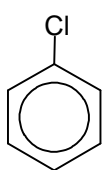
Naming aromatic compounds can be complicated. The simplest molecules are derivatives of benzene and have benzene at the root of the name



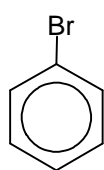
Methylbenzene



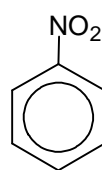
ethylbenzene



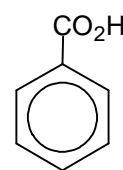
chlorobenzene



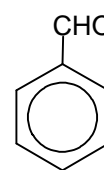
bromobenzene



nitrobenzene

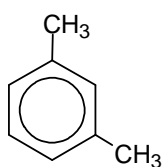


benzenecarboxylic acid

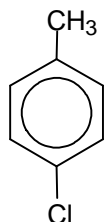


benzaldehyde

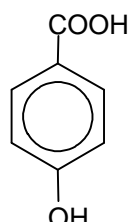
If two or more substituents are present on the benzene ring, their positions must be indicated by the use of numbers. This should be done to give the lowest possible numbers to the substituents. When two or more different substituents are present, they are listed in alphabetical order and di, tri prefixes should be used.



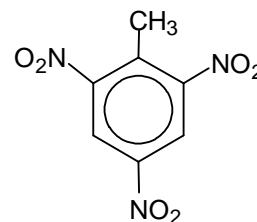
1,3-dimethylbenzene



1-chloro-4-methylbenzene

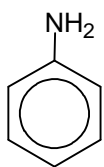


4-hydroxybenzenecarboxylic acid

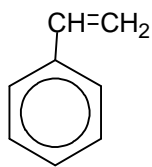


2,4,6-trinitromethylbenzene

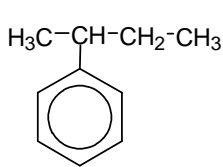
In other molecules the benzene ring can be regarded as a substituent side group on another molecule, like alkyl groups are. The C_6H_5 - group is known as the **phenyl** group.



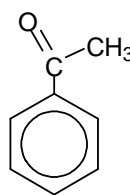
phenylamine



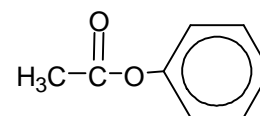
phenylethene



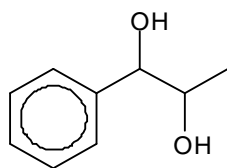
2-phenylbutane



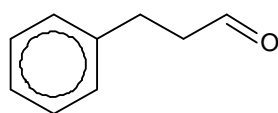
phenylethanone



phenylethanoate



1-phenylpropane-1,2-diol

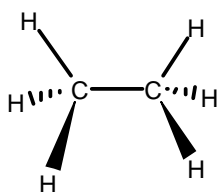


3-phenylpropanal

Shapes of organic molecules; σ and π bonds

Ethane C_2H_6

Each carbon in ethane has four σ bonds. They are arranged in a tetrahedral way around the carbon. The bond angle is 109.5°

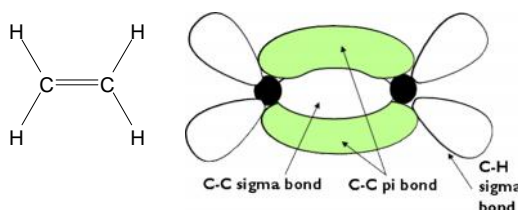


This is the shape and bond angle of any saturated hydrocarbon

Ethene C_2H_4

Each carbon in ethene forms two σ bonds to hydrogens.

C=C double covalent bond consists of **one sigma (σ) bond and one pi (π) bond.**



The arrangement of bonds around the $>C=C<$ is **planar** and each bond has the bond angle **120°**

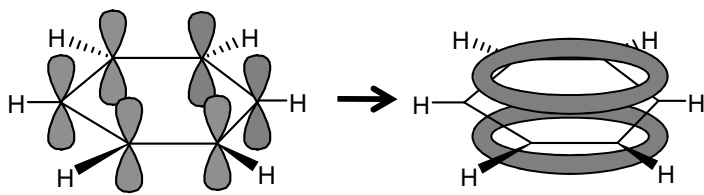
Carbonyls also have the same planar arrangement of bonds with a 120° bond angle

Benzene's Structure

The simplest arene is benzene. It has the molecular formula C_6H_6 . Its basic structure is six C atoms in a hexagonal ring, with one H atom bonded to each C atom.

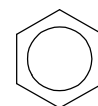
Each C atom is bonded to two other C atoms and one H atom by single covalent σ -bonds. This leaves one unused electron on each C atom in a p orbital, perpendicular to the plane of the ring.

The Six p electrons are delocalised in a ring structure above and below the plane of carbon atoms.

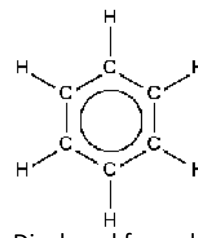


Benzene is a **planar** molecule. The evidence suggests all the C-C bonds are the same and have a length and bond energy between a C-C single and C=C double bond.

In formulae we draw a circle to show this delocalised system.



Abbreviated formula



Displayed formula

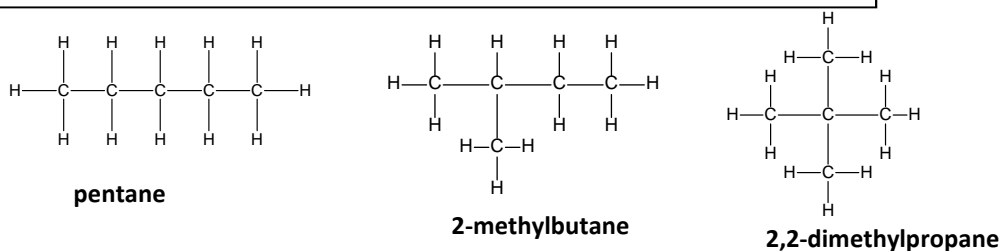
Isomers

Structural isomers: same molecular formula different structures (or structural formulae)

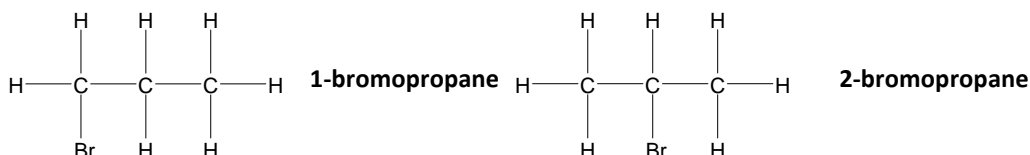
Structural isomerism can arise from

- Chain isomerism
- Position isomerism
- Functional group isomerism

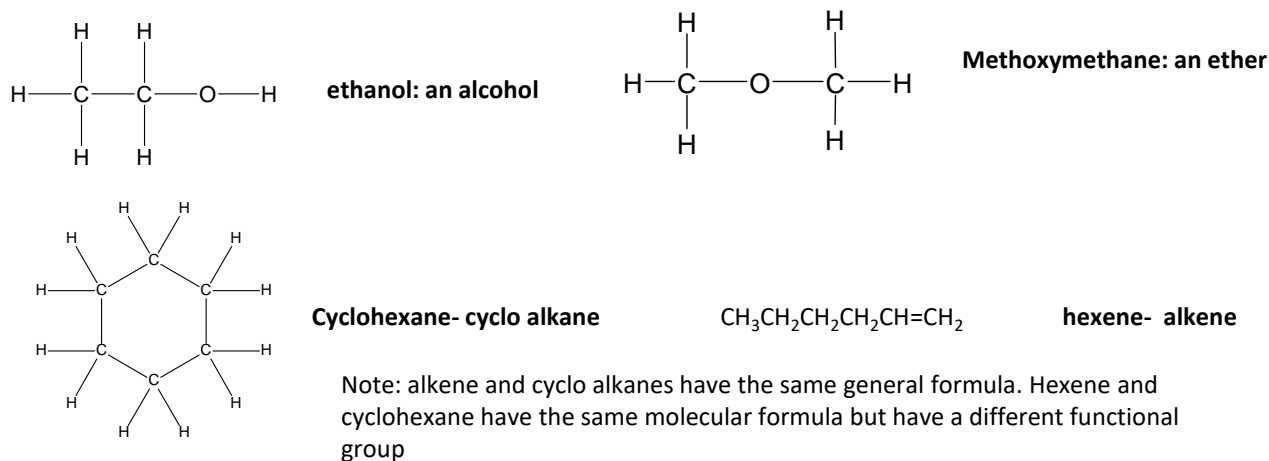
Chain isomers: Compounds with the same molecular formula but different structures of the carbon skeleton



positional isomers: Compounds with the same molecular formula but different structures due to different positions of the same functional group on the same carbon skeleton

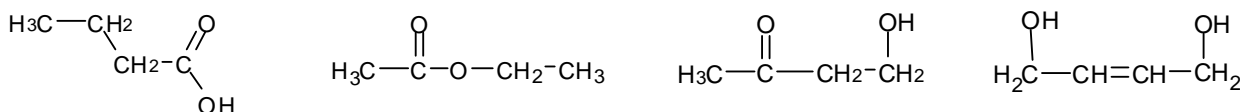


Functional group isomers: Compounds with the same molecular formula but with atoms arranged to give different functional groups



Aldehydes and ketones of the same chain length would be classed as functional group isomers- e.g. Propanal and propanone (both C₃H₆O)

Questions often involve functional group isomers of carboxylic acids: including esters etc



Stereoisomerism

Stereoisomers have the same structural formulae but have a different spatial arrangement of atoms.

Geometrical (cis-trans) isomerism

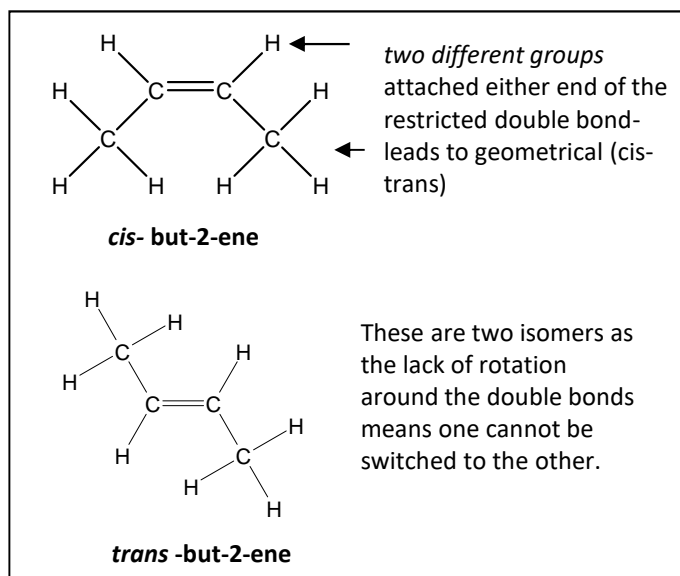
Alkenes can exhibit a type of isomerism called **Geometrical (cis-trans) isomerism**

Geometrical (cis-trans) isomers exist due to restricted rotation about the C=C bond due to the presence of π bonds

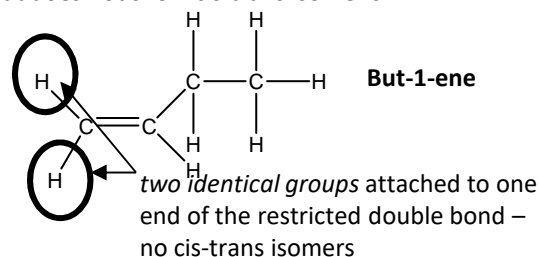
Single carbon-carbon covalent bonds can easily rotate

Geometrical (cis-trans) arise when:

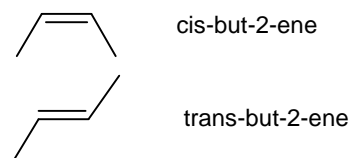
- There is **restricted rotation** around the C=C double bond.
- There are **two different groups/atoms** attached both ends of the double bond.



But-1-ene is a structural isomer of But-2-ene but does not show cis-trans isomerism.



Skeletal formulae can also represent E-Z isomerism

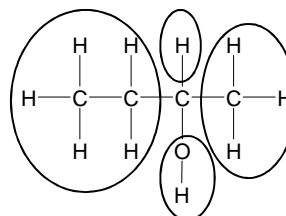


Optical Isomerism

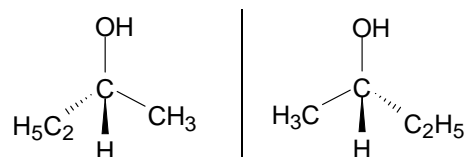
The second type of **stereoisomerism**: is optical isomerism

Optical isomerism occurs in carbon compounds with 4 different groups of atoms attached to a carbon (called an **asymmetric carbon**).

These four groups are arranged tetrahedrally around the carbon.



A carbon atom that has four different groups attached is called a **chiral** (asymmetric) carbon atom



This causes two different isomers that are not superimposable to be formed. They are mirror images

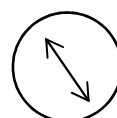
Many naturally occurring molecules contain chiral C atoms, but are usually found in nature as a pure enantiomer

Two compounds that are optical isomers of each other are called **enantiomers**.

Optical isomers have similar physical and chemical properties, but they rotate plane polarised light in different directions.

One enantiomer rotates it in one direction and the other enantiomer rotates it by **the same amount in the opposite direction**.

One optical isomer will rotate light clockwise (+)(called dextrorotatory). The other will rotate it anticlockwise(-)(called laevorotatory).



-ve enantiomer
Anticlockwise
rotation



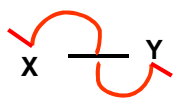
+ve enantiomer
clockwise rotation

Introduction to Mechanisms

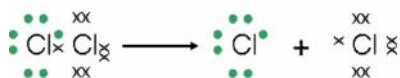
To understand how the reaction proceeds we must first understand how bonds are broken in organic mechanisms
There are two ways to break a covalent bond:

1. HOMOLYTIC FISSION:

each atom gets one electron from the covalent bond



one headed arrow shows movement of one electron



The bond has broken in a process called **homolytic** fission.

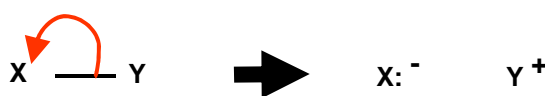
When a bond breaks by homolytic fission it forms two **Free Radicals**.

Free Radicals do not have a charge and are represented by a \cdot

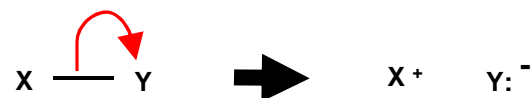
DEFINITION

A **Free Radical** is a reactive species which possess an **unpaired electron**

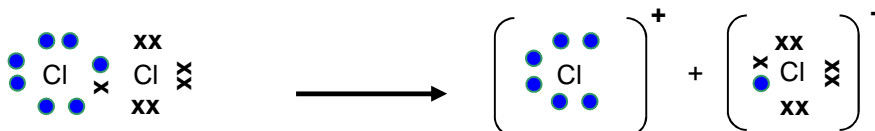
2. HETEROLYTIC FISSION: (*one atom gets both electrons*)



OR



two headed arrow shows movement of pair of electrons



Heterolytic fission produces **IONS**

Most organic reactions occur via heterolytic fission, producing ions

The Mechanism:

To understand a reaction fully we must look in detail at how it proceeds step by step. This is called its **mechanism**

We use curly arrows in mechanisms to show the movement of an electron pair showing either breaking or formation of a covalent bond;

A curly arrow will always **start** from a **lone pair** of electrons or the **centre of a bond**

The formation of a covalent bond is shown by a curly arrow that starts from a **lone electron pair** or from **another covalent bond**

The breaking of a covalent bond is shown by a curly arrow starting from the bond.

