3.1 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**

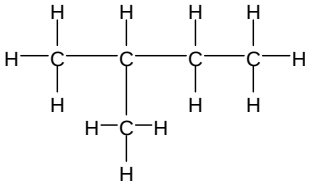
Empirical formula: shows the simplest whole number ratio of atoms of each element in the compound

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 $CH_3(CH_2)_2CH_3$,

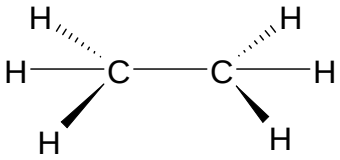
Displayed formula: show all the covalent bonds and atoms present in a molecule

Drawing displayed formulae

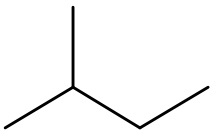


When drawing organic compounds add the hydrogen atoms so that each carbon has 4 bonds

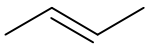
Remember that the shape around the carbon atom in saturated hydrocarbons is tetrahedral and the bond angle is 109.5°



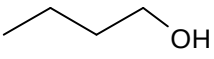
Skeletal formula shows the simplified organic formula, shown by removing hydrogen atoms from alkyl chains, leaving just a carbon skeleton and associated functional groups.



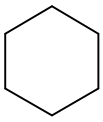
2-methylbutane



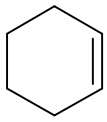
But-2-ene



Butan-1-ol



cyclohexane

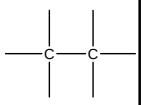
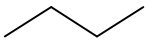
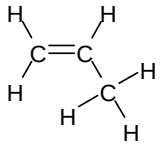
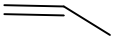
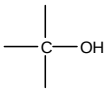
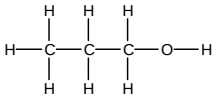
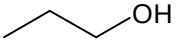
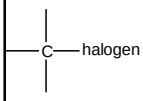
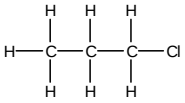
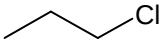
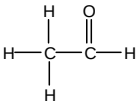
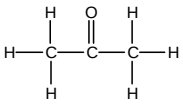
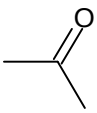
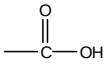
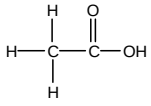
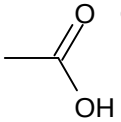
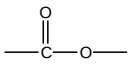
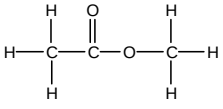
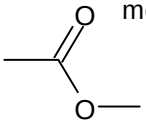


cyclohexene

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.

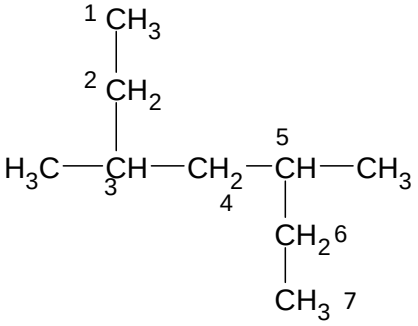
homologous series	functional group	prefix / suffix (* = usual use)	example
Alkane		*-ane*	$CH_3CH_2CH_2CH_3$  butane
Alkenes		*Suffix** **-ene**	  propene
Alcohols		*suffix** **-ol** *prefix* **hydroxy-**	 propan-1-ol 
Halogenoalkanes		*Prefix** **chloro-** **bromo-** **iodo-**	 1-chloropropane 
Aldehydes		*suffix* **-al** *prefix* **formyl-**	  ethanal
Ketones		*suffix** *-o***ne** *prefix* **oxo-**	  propanone
Carboxylic acids		*suffix** **-oic acid**	  ethanoic acid
Esters		*-yl –oate*	  methylethanoate

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 (and the lowest number on the carbon chain), 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 >aldehydes>ketones>alcohols>alkenes>halogenoalkanes

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 $-CH_3$ methyl or $-C_2H_5$ ethyl $-C_3H_7$ propyl



3,5-dimethylheptane

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

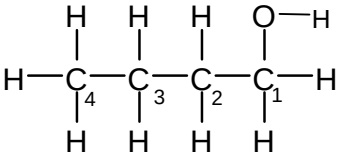
The functional group is named by a prefix or suffix. e.g. **bromo**ethane, ethan**ol**, prop**ene**

- 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

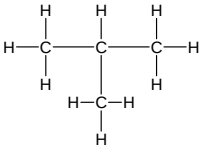
  If the suffix starts with a consonant or there are two or more of a functional group meaning di, or tri needs to be used then **do not remove the the –e** from the stem alkane name
  e.g. Propan**e**nitrile, ethan**e**-1,2-diol, propan**e**dioic acid, propan**e**-1,2,3-triol, pentan**e**-2,4-dione.

- 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.



Butan-1-ol

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



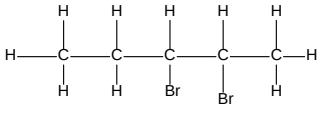
methylpropane

$CHCl_3$ trichloromethane

- 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



2,3-dibromopentane.

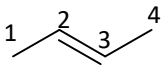
- Words are separated by numbers with dashes
- numbers are separated by commas
- If there is more than one functional group or side chain, the groups are listed in alphabetical order (ignoring any *di*, *tri*).

$CH_2FCCl_2CH_2CH_3$ 2,2-dichloro-1-fluorobutane.

$CH_2FCH_2CHBrCH_2CH_3$ 3-bromo-1-fluoropentane

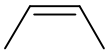
Alkenes

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



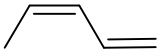
Double bond between C^2 and C^3 so But-2-ene

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



Z-but-2-ene

If more than one double bond is present then suffix ends **di**ene or **tri**ene. The stem ends in **a**

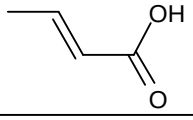


Pent**a**-1,3-diene

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

$CH_2OHCHBrCH=CH_2$

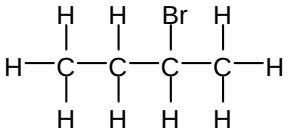
2-bromobut-3-**en**-1-ol



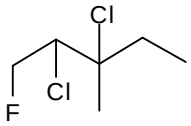
E-but-2-**en**oic acid

Halogenoalkanes

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

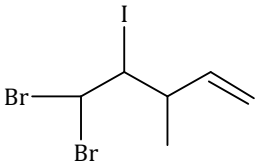


2-bromobutane



2,3-dichloro-1-fluoro-3-methylpentane

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

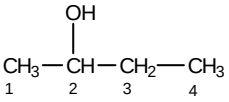


5,5-dibromo-4-iodo-3-methylpent-1-ene

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

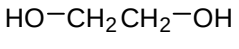
Alcohols

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

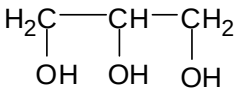


Butan-2-ol

If there are two or more -OH groups then di, tri are used.
Add the **'e'** on to the stem name though.

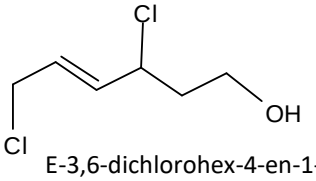


Ethan**e**-1,2-diol



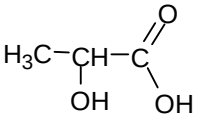
propan**e**-1,2,3-triol

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



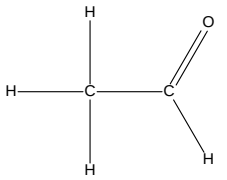
E-3,6-dichlorohex-4-en-1-ol

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-**:



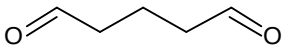
2-hydroxypropanoic acid

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 carbon on the chain.



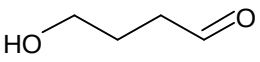
ethan**al**

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.

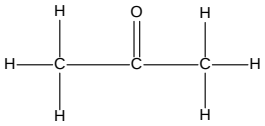


4-hydroxybutanal

Ketones

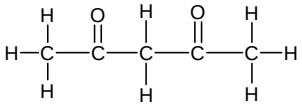
Ketones end in **-one**

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



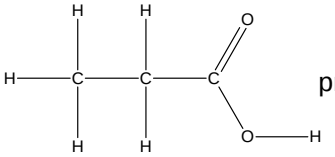
propan**one**

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



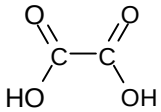
pentan**e**-2,4-dione

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.



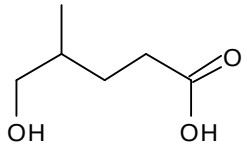
propan**oic acid**

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



ethan**edioic acid**

Note the **e** in this name



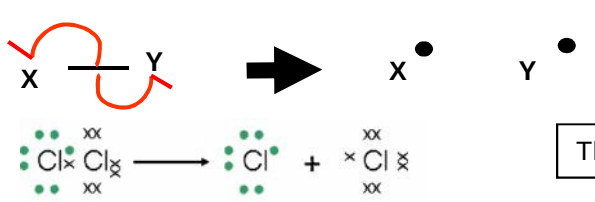
5-hydroxy-4-methylpentanoic acid

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.

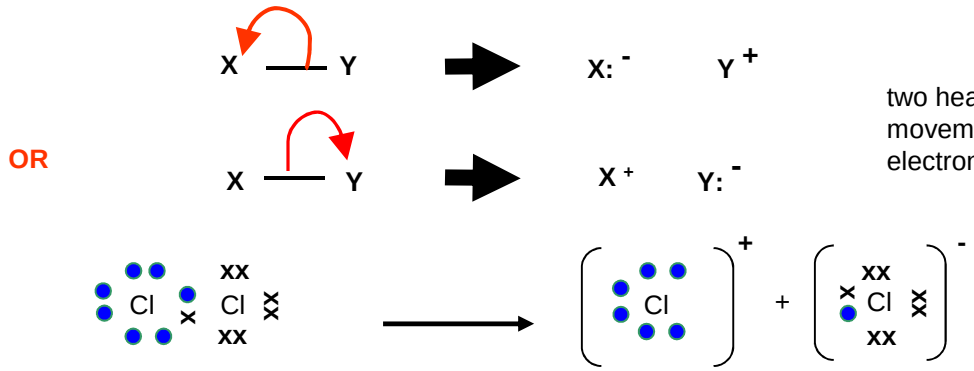
When a bond breaks by homolytic fission it forms two **free radicals.**

Free radicals do not have a charge and are represented by a •

Definition

A **free radical** is a reactive species which possess an **unpaired electron**

2. Heterolytic fission: (***one*** *atom gets* ***both*** *electrons*)



two headed arrow shows movement of pair of electrons

Heterolytic fission produces **ions**

Most organic reactions occur via heterolytic fission, producing ions

The mechanism:

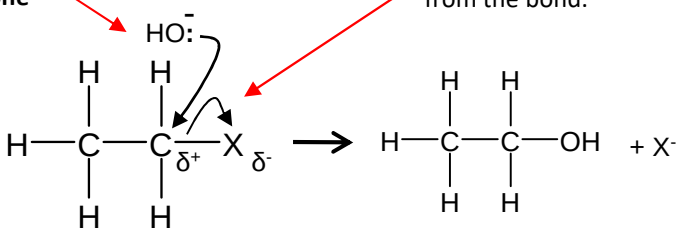
To understand a reaction fully we must look in detail at how it proceeds step by step. This is called its **mechanism**

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.



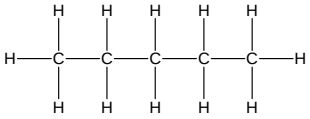
Isomers

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

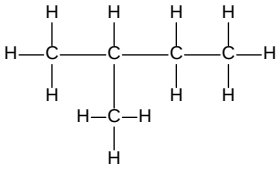
Structural isomerism can arise from

- Chain isomerism
- Position isomerism
- Functional group isomerism

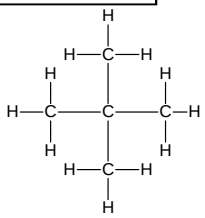
Chain isomers: Compounds with the same molecular formula but different structures of the carbon skeleton



pentane

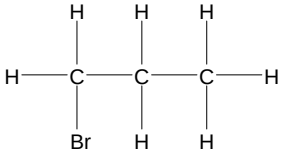


2-methylbutane

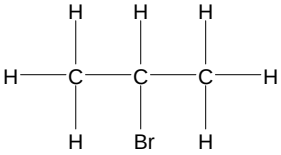


2,2-dimethylpropane

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

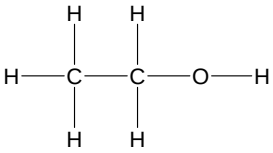


1-bromopropane

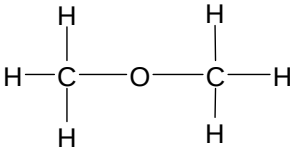


2-bromopropane

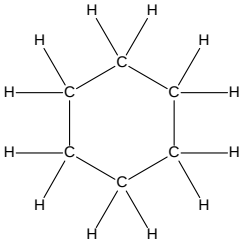
Functional group isomers: Compounds with the same molecular formula but with atoms arranged to give different functional groups



ethanol: an alcohol



Methoxymethane: an ether



cyclohexane- cyclo alkane

$CH_3CH_2CH_2CH_2CH=CH_2$ **hexene- alkene**

Note: alkene and cyclo alkanes have the same general formula. Hexene and cyclohexane have the same molecular formula but have a different functional group

Stereoisomerism

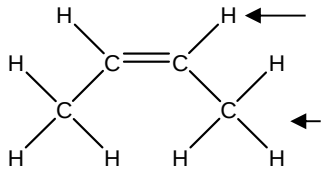
Stereoisomers have the same structural formulae but have a different spatial arrangement of atoms.

Alkenes can exhibit a type of isomerism called **E-Z stereoisomerism**

E-Z isomers exist due to restricted rotation about the C=C bond

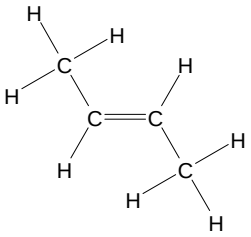
Single carbon-carbon covalent bonds can easily rotate

E-Z stereoisomers arise when:
(a) There is **restricted rotation** around the C=C double bond.
(b) There are **two different groups/atoms** attached both ends of the double bond.



two different groups attached either end of the restricted double bond- leads to EZ isomers

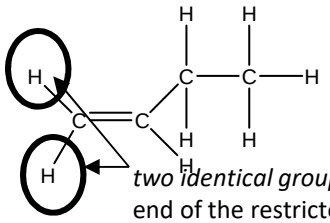
***Z*- but-2-ene**



These are two isomers as the lack of rotation around the double bonds means one cannot be switched to the other.

***E* -but-2-ene**

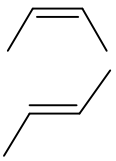
But-1-ene is a structural isomer of But-2-ene but does not show E-Z isomerism.



But-1-ene

two identical groups attached to one end of the restricted double bond – no E-Z isomers

Skeletal formulae can also represent E-Z isomerism



Z-but-2-ene

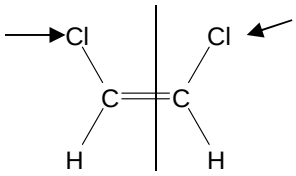
E-but-2-ene

Naming E-Z stereoisomers

First determine the priority groups on both sides of the double bond

Priority Group: The atom with the bigger atomic number is classed as the priority atom

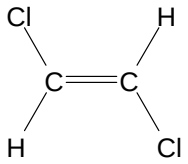
Priority group side 1



Priority group side 2

Z-1,2-dichloroethene

If the priority atom is on the same side of the double bond it is labelled Z from the german zusammen (The Zame Zide!)



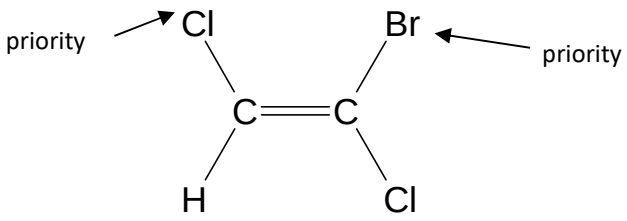
E-1,2-dichloroethene

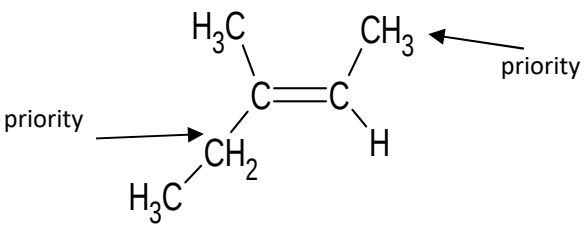
If the priority atom is on the opposite side of the double bond it is labelled E from the german entgegen (The Epposite side!)

Cahn–Ingold–Prelog (CIP) priority rules.

1. Compare the atomic number of the atoms directly attached to each side of the double bond; the atom of higher atomic number is given priority.

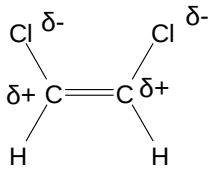
2. If the atoms are the same, consider the atoms at distance 2 from the double bond. Make a list of each atom bonded to the one directly attached to the double bond. Arrange list in order of decreasing atomic number. Compare the lists atom by atom; at the earliest difference, the group containing the atom of higher atomic number is given priority



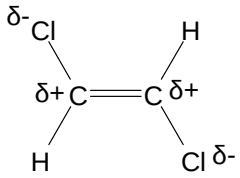


The effect of EZ stereoisomerism on physical properties

E-Z stereoisomers can have differing melting and boiling points.



Z-1,2-dichloroethene
Boiling point =60°C
This molecule is **polar**. The polar C-Cl bonds are on the same side of the molecule. One side of the molecule is slightly negative.
The intermolecular forces are both van der waals and permanent dipole-dipole attractions.



E-1,2-dichloroethene
Boiling point =48°C
This molecule is non- **polar**. The polar C-Cl bonds are on opposite sides of the molecule. The dipoles cancel out.
The intermolecular forces are only van der waals so lower boiling point.