# 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**

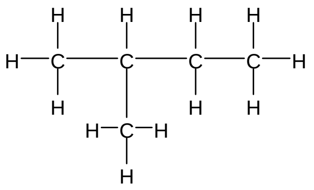
**Empirical formula**: shows the simplest whole number ratio of atoms of each element in the compound

**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 $CH_3(CH_2)_2CH_3$,

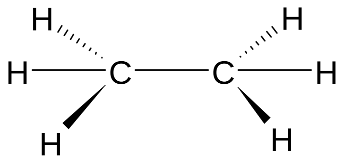
**Displayed formula**: show all the covalent bonds and atoms present in a molecule

### Drawing Displayed formulae

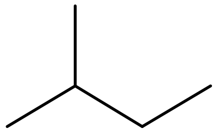


When drawing organic compounds add the hydrogen atoms so that each carbon has 4 bonds

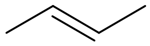
Remember that the shape around the carbon atom in saturated hydrocarbons is tetrahedral and the bond angle is 109.5°



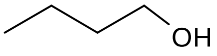
**Skeletal formula** shows the simplified organic formula, shown by removing hydrogen atoms from alkyl chains, leaving just a carbon skeleton and associated functional Groups.



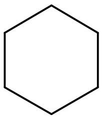
2-methylbutane



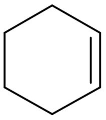
But-2-ene



Butan-1-ol



cyclohexane

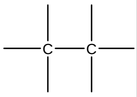
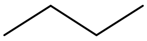
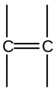
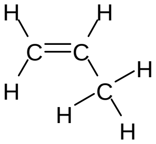
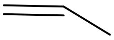
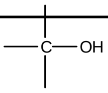
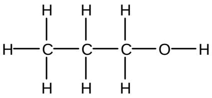
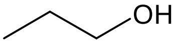
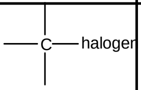
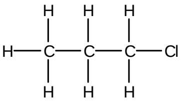
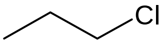
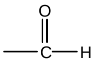
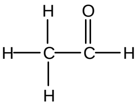
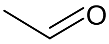
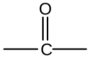
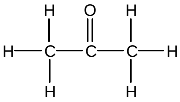
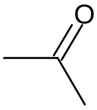
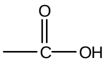
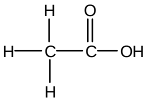
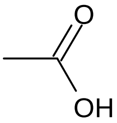
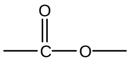
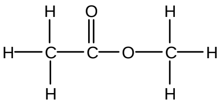
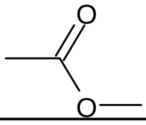


cyclohexene

**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.

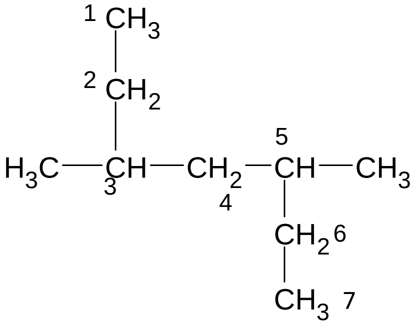
**Functional group** is an atom or group of atoms which when present in different molecules causes them to have similar chemical properties

| homologous series | functional group | prefix / suffix (* = usual use) | example |
|---|---|---|---|
| Alkane |  | *-ane* | $CH_3CH_2CH_2CH_3$  Butane |
| Alkenes |  | *suffix* **-ene** |   propene |
| Alcohols |  | *suffix** **-ol**<br>*prefix* **hydroxy-** |  Propan-1-ol  |
| Halogenoalkanes |  | *prefix* **chloro-**<br>**bromo-**<br>**iodo-** |  1-chloropropane  |
| Aldehydes |  | *suffix* **-al**<br>*prefix* **formyl-** |   ethanal |
| Ketones |  | *suffix** *-o***ne**<br>*prefix* **oxo-** |   Propanone |
| carboxylic acids |  | *suffix* **-oic acid** |   Ethanoic acid |
| Esters |  | *-yl –oate* | methylethanoate   |

### 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**

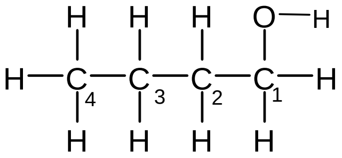
The functional group is named by a prefix or suffix. e.g. **bromo**ethane, ethan**ol**, prop**ene**

- 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

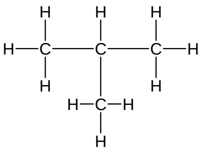
If the suffix starts with a consonant or there are two or more of a functional group meaning di, or tri needs to be used then **do not remove the the –e** from the stem alkane name
e.g. Propan**e**nitrile, ethan**e**-1,2-diol, propan**e**dioic acid, propan**e**-1,2,3-triol, Pentan**e**-2,4-dione.

- 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.



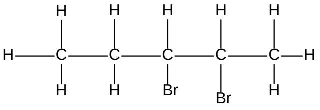
methylpropane

$CHCl_3$ 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.

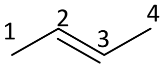
- Words are separated by numbers with dashes
- numbers are separated by commas
- If there is more than one functional group or side chain, the groups are listed in alphabetical order (ignoring any *di*, *tri*).

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

$CH_2FCH_2CHBrCH_2CH_3$ 3-bromo-1-fluoropentane

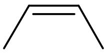
### Alkenes

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



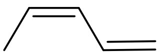
Double bond between $C^2$ and $C^3$ so But-2-ene

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



Z-but-2-ene

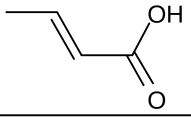
If more than one double bond is present then suffix ends **di**ene or **tri**ene. The stem ends in **a**



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

The suffix for alkenes can go in front of other suffixes.

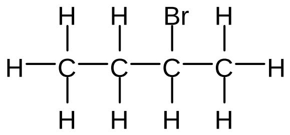
$CH_2OHCHBrCH=CH_2$ 2-bromobut-3-**en**-1-ol



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

### Halogenoalkanes

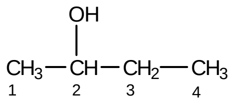
Class the halogen as a substituent on the C chain and use the suffix **-fluoro**, **-chloro**, **-bromo**, or **–iodo**. (Give the position number if necessary)



2-bromobutane

### Alcohols

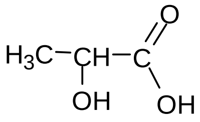
These have the ending **-ol** and if necessary the position number for the OH group is added between the name stem and the –ol



$CH_3-CH(OH)-CH_2-CH_3$

Butan-2-ol

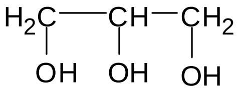
If the compound has an –OH group in addition to other functional groups that need a suffix ending then the OH can be named with the prefix **hydroxy-**:



2-hydroxypropanoic acid

$HO-CH_2CH_2-OH$ Ethan**e**-1,2-diol

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

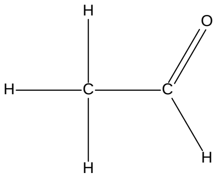


$H_2C(OH)-CH(OH)-CH_2(OH)$

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

### 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.

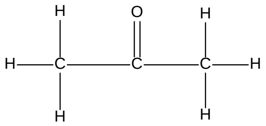


Ethan**al**

### Ketones

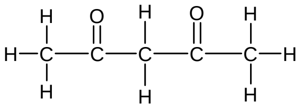
Ketones end in **-one**

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**

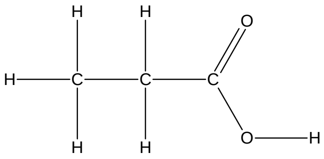
If two ketone groups then **di** is put before **–one** and an an **e** is added to the stem.



Pentan**e**-2,4-dione

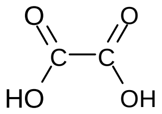
### Carboxylic acids

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



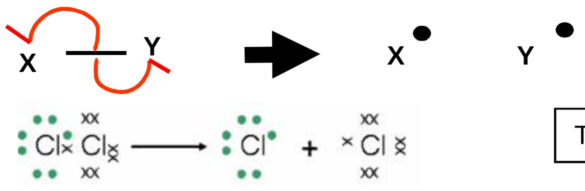
Ethan**edioic acid**

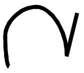
Note the **e** in this name

## 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.

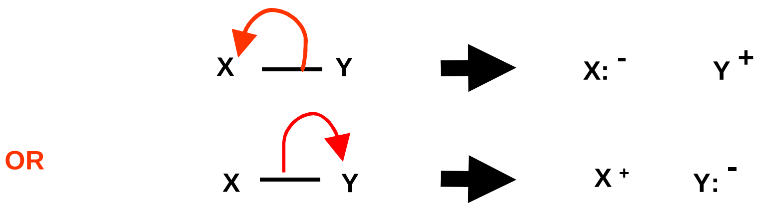
When a bond breaks by homolytic fission it forms two **Free Radicals.**

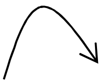
**Free Radicals** do not have a charge and are represented by a •

**DEFINITION**

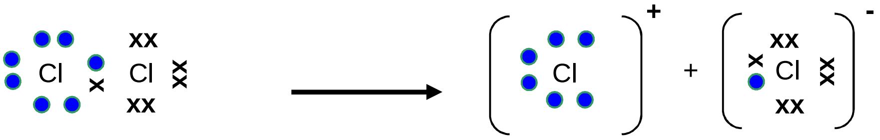
A **Free Radical** is a reactive species which possess an **unpaired electron**

**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

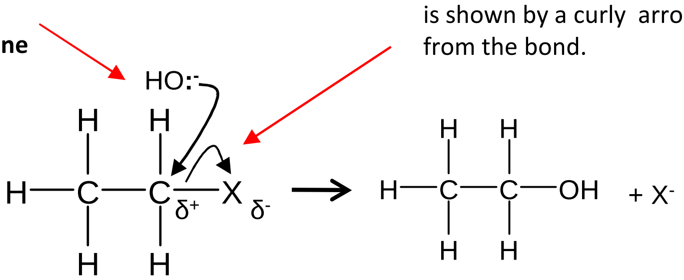
**The Mechanism**: To understand a reaction fully we must look in detail at how it proceeds step by step. This is called its **mechanism**

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.



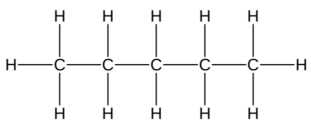
## Isomers

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

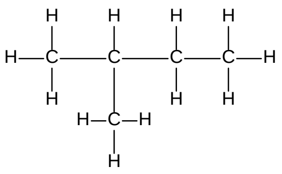
Structural isomerism can arise from

- Chain isomerism
- Position isomerism
- Functional group isomerism

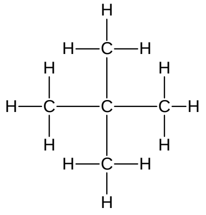
**Chain isomers**: Compounds with the same molecular formula but different structures of the carbon skeleton



**pentane**

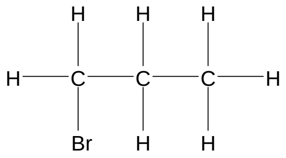


**2-methylbutane**

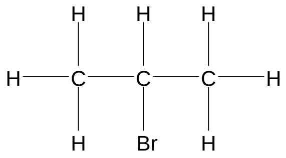


**2,2-dimethylpropane**

**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

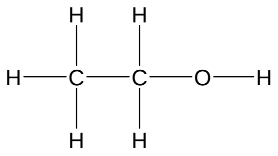


**1-bromopropane**

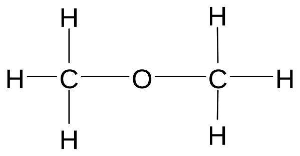


**2-bromopropane**

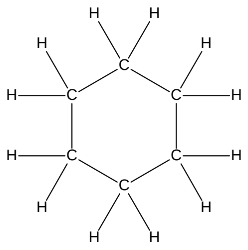
**Functional group isomers**: Compounds with the same molecular formula but with atoms arranged to give different functional groups



**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

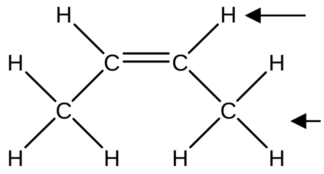
Stereoisomers have the same structural formulae but have a different spatial arrangement of atoms.

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

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

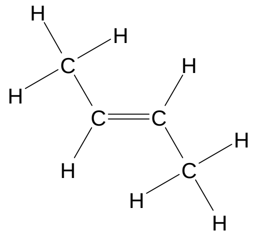
Single carbon-carbon covalent bonds can easily rotate

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

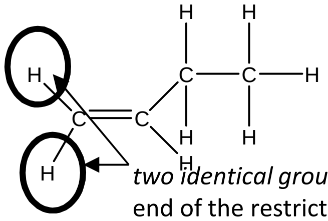
***Z*- but-2-ene**



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**

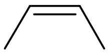
But-1-ene is a structural isomer of But-2-ene but does not show E-Z isomerism.



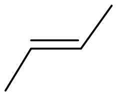
**But-1-ene**

*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

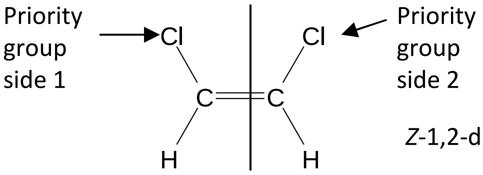


E-but-2-ene

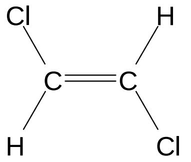
**Naming E-Z stereoisomers**

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



*Z*-1,2-dichloroethene



*E*-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!)

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