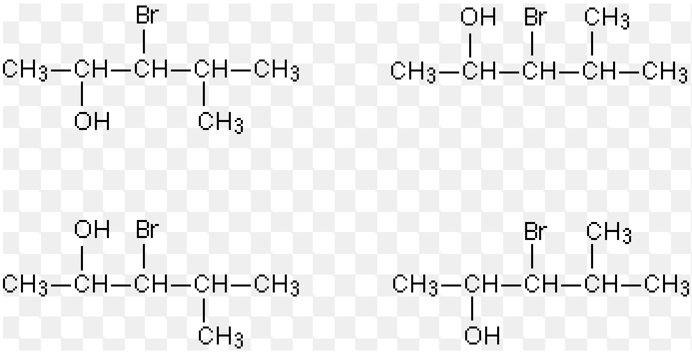
UNIT 7

INTRODUCTION TO ORGANIC CHEMISTRY

PART 1 – NOMENCLATURE AND ISOMERISM IN SIMPLE ORGANIC MOLECULES



Contents

Key words: unbranched, branched, aliphatic, alicyclic, alkane, alkene, alkyne, haloalkane, alkanol, homologous series, structural isomerism, geometrical isomerism, stereoisomerism

1) Overview

- Organic chemistry is the chemistry of carbon compounds. Carbon forms a vast number of compounds because it can form strong covalent bonds with itself. This enables it to form long chains (up to 5000 in length) of carbon atoms, and hence an almost infinite variety of carbon compounds are known.

- Most living organisms are composed largely of organic molecules. Organic Chemistry thus forms the basis for Biochemistry – the Chemistry of Living Organisms

- All organic compounds contain carbon. Most contain hydrogen. Some contain oxygen.

- In every molecule, each carbon atom always forms four covalent bonds. Each hydrogen atom always forms one covalent bond. Each oxygen atom always forms two covalent bonds.

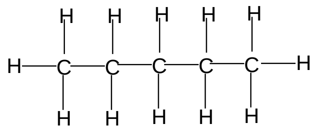
2) Describing and classifying organic molecules

When describing an organic molecule, there are two main things to consider:

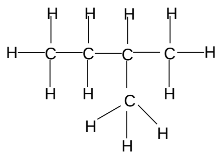
a) The number and arrangement of carbon atoms in the molecule.

The total number of carbon atoms in a molecule can vary from 1 to more than 1,000,000.

In many cases, all the carbon atoms are arranged in an **unbranched** chain. Often, however, molecules contain shorter chains of carbon atoms branching off a longer chain. These are known as **branched** molecules.

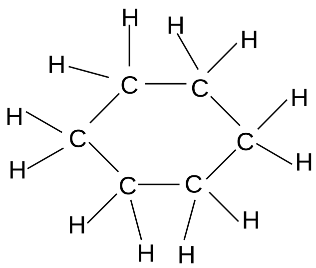


Unbranched molecule

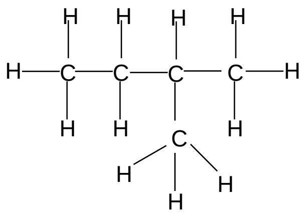


Branched molecule

Carbon atoms can also be arranged to form rings. These are known as **alicyclic** molecules. The most common number of carbon atoms in a ring is 6. Molecules which do not contain a ring are known as **aliphatic** molecules.



Alicyclic molecule

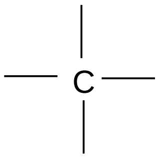
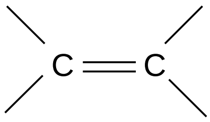
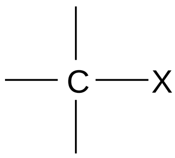
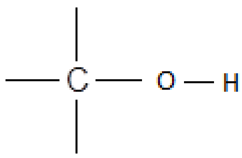


Aliphatic molecule

b) The functional groups in the molecule

A functional group is a specific atom or group of atoms which confer certain physical and chemical properties onto the molecule. Organic molecules are classified by the dominant functional group on the molecule.

These are the some of the most important functional groups found on organic molecules:

Type of compound	Nature of functional group
Alkane	C-C and C-H single bonds only (ie no functional group) 
Alkene	C=C double bond 
Alkyne	C≡C triple bond -C≡C-
Haloalkane -Chloroalkane -Bromoalkane -Iodoalkane	Cl, Br or I atom attached to a carbon atom 
Alcohol	O atom in between a C atom and an H atom 

Molecules which contain carbon and hydrogen only are known as **hydrocarbons**.

Alkanes, alkenes and alkynes are examples of hydrocarbons.

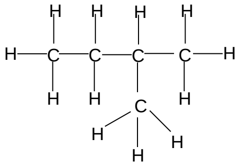
Haloalkanes and alcohols are not hydrocarbons.

3) Drawing and writing organic molecules

Organic compounds can be represented in a number of ways:

a) Displayed formula, showing all covalent bonds

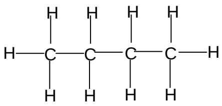
This is also known as the **graphical formula**. All covalent and ionic bonds between all atoms are shown:

eg 

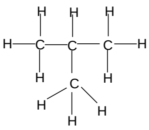
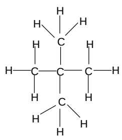
b) Structural formula, not showing covalent bonds

Enough information is shown to make the structure clear, but the actual covalent bonds are omitted.

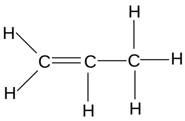
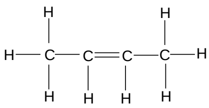
Unbranched alkanes are shown as follows:

 is represented as $CH_3CH_2CH_2CH_3$ or $CH_3(CH_2)_2CH_3$.

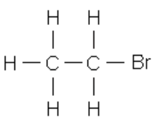
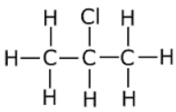
Branched alkanes are shown as follows:

 is represented as $CH_3CH(CH_3)CH_3$.  is represented as $CH_3C(CH_3)_2CH_3$.

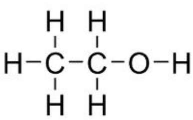
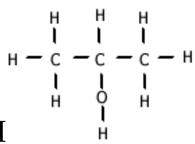
Alkenes are shown as follows:

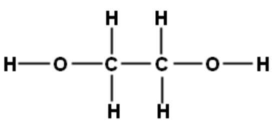
 is represented as CH_2CHCH_3.  is represented as $CH_3CHCHCH_3$.

Haloalkanes are represented as follows:

 is represented as CH_3CH_2Br  is represented as $CH_3CHClCH_3$

Alcohols are represented as follows:

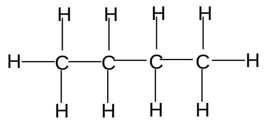
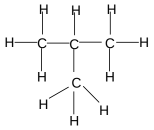
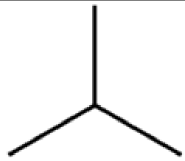
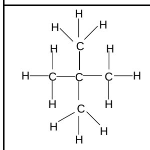
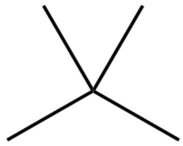
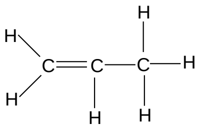
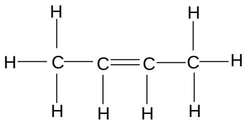
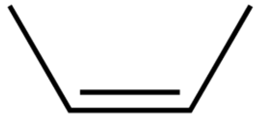
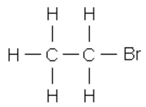
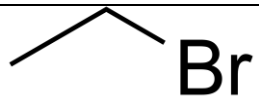
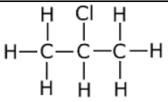
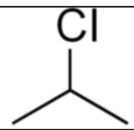
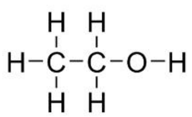
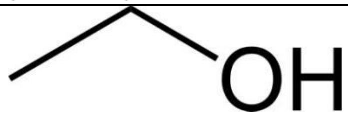
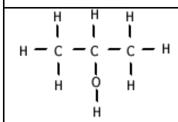
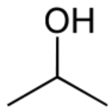
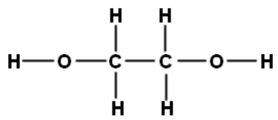
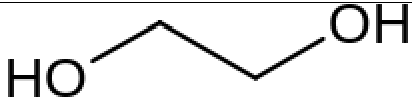
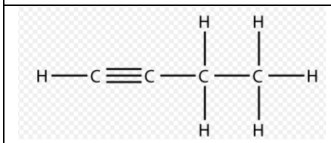
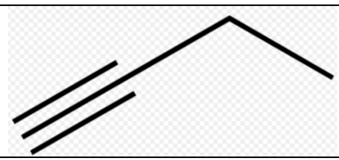
 is represented as CH_3CH_2OH  is represented as $CH_3CH(OH)CH_3$

 is represented as $HOCH_2CH_2OH$

c) Skeletal formula, not showing carbon atoms

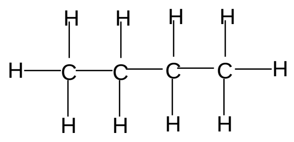
In skeletal formulae:

- carbon atoms are not drawn – they are represented by a dot
- hydrogen atoms are not drawn if they are bonded to carbon atoms
- covalent bonds are represented by a line if they do not involve hydrogen
- covalent bonds involving hydrogen are omitted
- the angle between the bonds must be correct

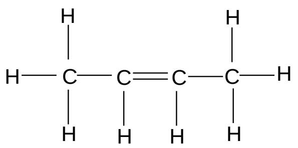
	is represented as	
	is represented as	
	is represented as	
	is represented as	
	is represented as	
	is represented as	
	is represented as	
	is represented as	
	is represented as	
	is represented as	
	is represented as	

d) Molecular formula

The molecular formula shows the number of each atom in one molecule of the compound. It does not show unequivocally the structure of the molecule, so different molecules can have the same molecular formula. **Molecules with the same molecular formula but different structures** are known as **isomers**.



is written C_4H_{10}



is written C_4H_8

Alkanes have the general molecular formula C_nH_{2n+2}.

Alkenes have the general molecular formula C_nH_{2n}.

Haloalkanes have the general molecular formula $C_nH_{2n+1}X$.

Alcohols have the general molecular formula $C_nH_{2n+2}O$.

e) Empirical formula

The empirical formula is the simplest whole number ratio of the number of atoms of each element in a substance.

Test Your Progress: Topic 7 Part 1 Exercise 1

1. Draw a compound with four carbon atoms which is:
   (a) an unbranched alkane
   (b) an alicyclic alcohol
   (c) a branched alkene
   (d) an unbranched alkyne
   (e) a dibromoalkane

2. Draw the displayed, structural, skeletal and molecular formula of a branched alcohol with five carbon atoms.

3. Deduce the general molecular formula of aliphatic alkynes

4) Nomenclature of organic molecules

Most organic compounds can be named systematically by the IUPAC method.

In order to describe completely an organic molecule, three features must be described:

- the longest unbranched carbon chain on the molecule.
- the length and position of any branches on the molecule.
- the nature and position of any functional groups on the molecule.

a) The longest unbranched chain on the molecule

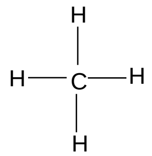
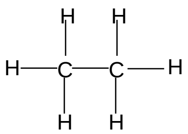
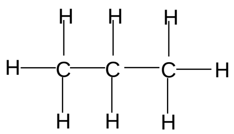
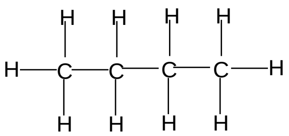
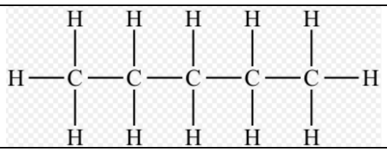
The longest carbon chain on the molecule is indicated by one of the following prefixes:

Number of carbon atoms in the chain	Prefix
1	Meth-
2	Eth-
3	Prop-
4	But-
5	Pent-

b) The nature and position of any functional groups on the molecule

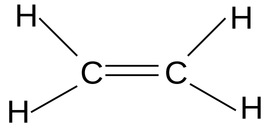
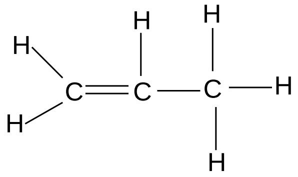
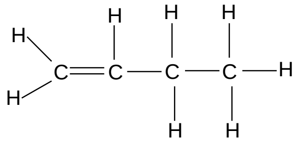
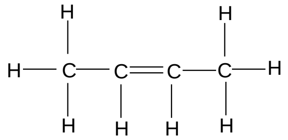
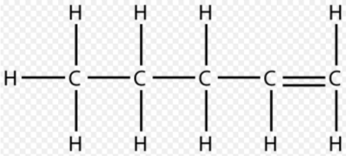
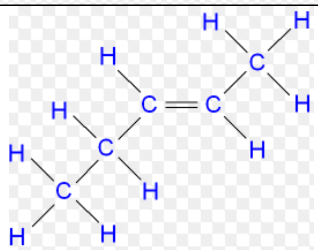
(i) Alkanes

Alkanes are named using the ending -ane:

	Methane
	Ethane
	Propane
	Butane
	Pentane

(ii) Alkenes

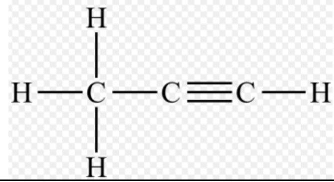
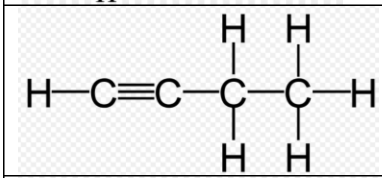
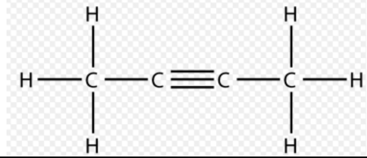
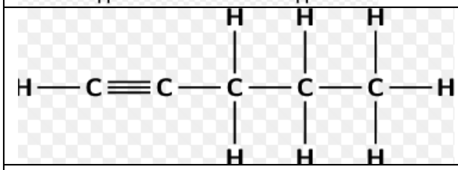
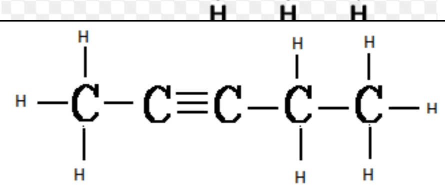
Alkenes are named using the ending -ene. In molecules with an unbranched chain of 4 or more carbon atoms, the position of the C=C double bond must be specified. The carbon atoms on the unbranched chain must be numbered, starting with the end closest to the double bond. The lowest-numbered carbon atom participating in the double bond is indicated just before the -ene:

	Ethene
	Propene
	But-1-ene
	But-2-ene
	Pent-1-ene
	Pent-2-ene

Note that pent-1-ene and pent-2-ene have the same molecular formula, but different structures. This means that they are **isomers** of each other. But-1-ene and but-2-ene are also isomers of each other.

(iii) Alkynes

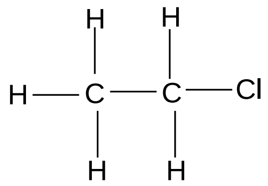
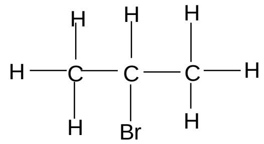
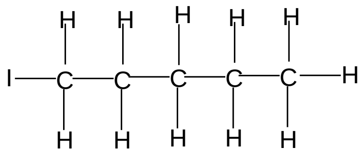
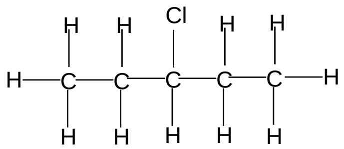
Alkynes are named using the ending -yne. In molecules with an unbranched chain of 4 or more carbon atoms, the position of the C≡C triple bond must be specified. The rules to be followed are the same as in alkenes:

$H-C\equiv C-H$	Ethyne
	Propyne
	But-1-yne
	But-2-yne
	Pent-1-yne
	Pent-2-yne

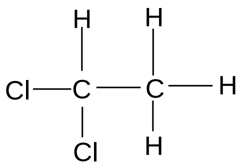
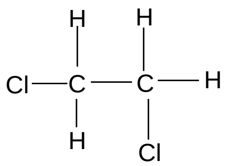
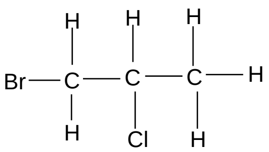
Note that pent-1-yne and pent-2-yne have the same molecular formula, but different structures. This means that they are **isomers** of each other. But-1-yne and but-2-yne are also isomers of each other.

(iv) **Haloalkanes**

Haloalkanes are named using the prefix chloro-, bromo- or iodo-, with the ending -ane. In molecules with an unbranched chain of three or more carbon atoms, the position of the halogen atom must also be specified. The carbon atoms on the straight chain must be numbered, starting with the end closest to the halogen atom. The number of the carbon atom attached to the halogen is indicated before the prefix:

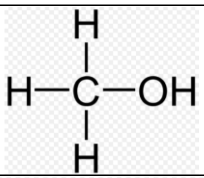
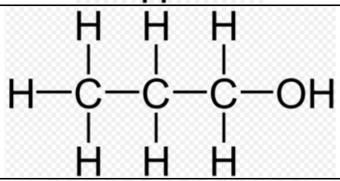
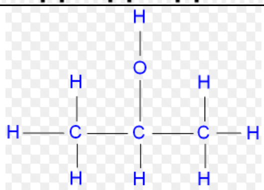
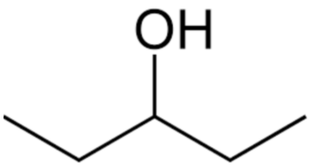
	Chloroethane
	2-bromopropane
	1-iodopentane
	3-chloropentane

The position of all halogens in dihaloalkanes except those with one carbon atom must be specified. If there is more than one of the same type of halogen atom on the molecule, the di (two), tri (three) or tetra (four) prefixes must also be used.

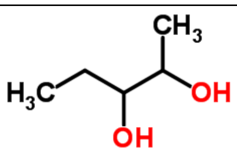
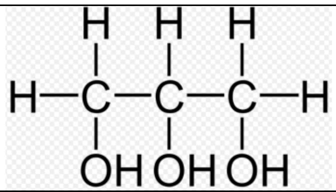
	1,1-dichloroethane
	1,2-dichloroethane
	1-bromo,2-chloropropane

(v) Alcohols

Alcohols are named using the ending -anol. In molecules with an unbranched chain of three or more carbon atoms, the position of the functional group must also be specified. The carbon atoms on the unbranched chain must be numbered, starting with the end closest to the OH group. The number of the carbon atom attached to the oxygen is indicated in between the an and the ol:

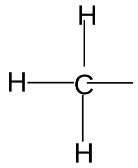
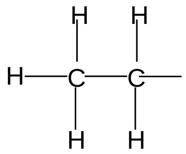
	Methanol
	Propan-1-ol
	Propan-2-ol
	Pentan-3-ol

The position of all OH groups in diols except those with one carbon atom must be specified. The di (two), tri (three) or tetra (four) prefixes must also be used.

HO-CH_2-CH_2-OH	Ethan-1,2-diol
$HOCH_2CH_2CH_2OH$	Propan-1,3-diol
	Pentan-2,3-diol
	Propan-1,2,3-triol

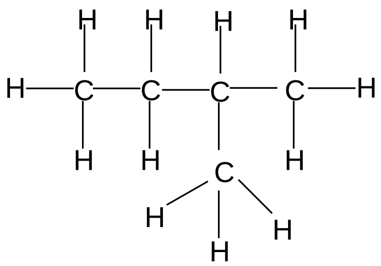
c) The length and position of any branches on the molecule

Many carbon chains are branched. The presence of a branch is indicated one of the following prefixes:

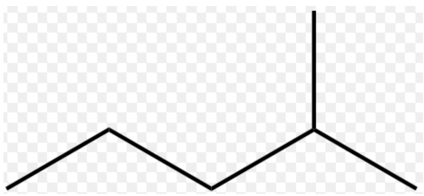
Branch	Prefix
	Methyl
	Ethyl

In some cases, there is more than one place in which the branch can be attached. In such cases, the position of the branch must be specified according to the number of the carbon on the straight chain to which it is attached. The carbons are always numbered from the carbon at the end of the chain closest to the functional group. If there is no functional group, the carbons are numbered from the carbon at the end of the chain closest to the branch.

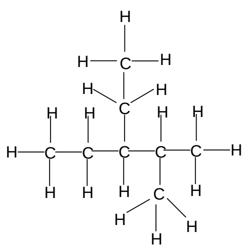
Eg



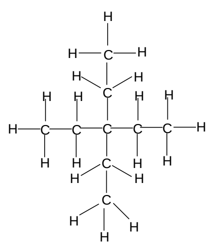
methylbutane



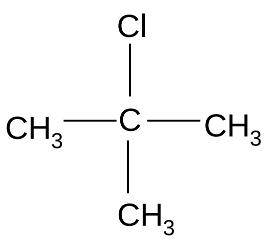
2-methylpentane



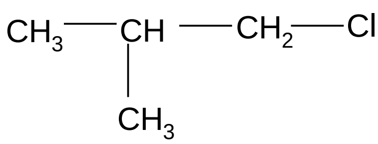
2-methyl,3-ethylpentane



diethylpentane



2-chloromethylpropane



1-chloromethylpropane

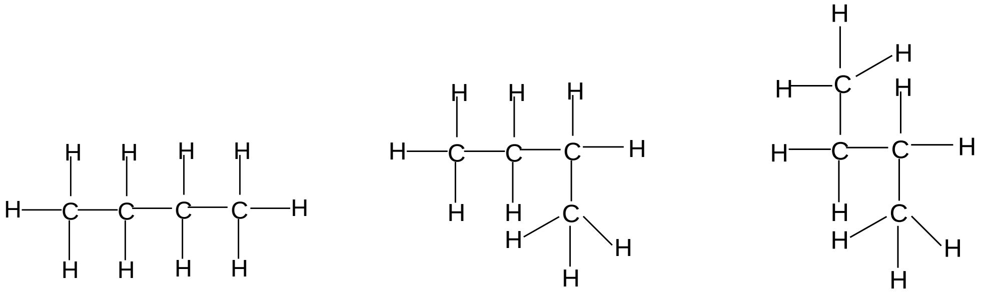
5) Recognising Identical Organic Molecules

Many organic compounds which appear to be different are in fact the same. They appear to be different because different notations are used, or because some of the bonds are simply rotated.

All single covalent bonds are able to rotate freely.

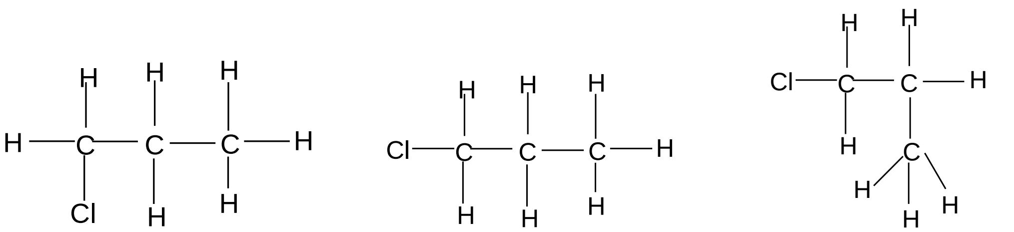
Eg butane can be represented in a number of ways:

Such as



Eg 1-chloropropane can be represented in a number of ways:

Such as

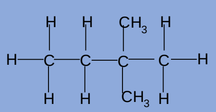


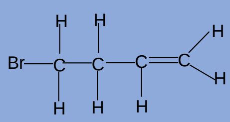
All molecules which are identical must have the same name and all molecules with the same name must be identical.

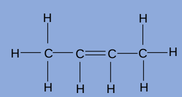
Two non-identical molecules cannot have the same name.

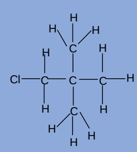
Test Your Progress: Unit 7 Part 1 Exercise 2

1. Name the following compounds:









$CH_3CH(CH_3)CH_3$ $CH_3CHBrCH_2Br$ $CH_2=CHCH_2CH_3$ $CH_3CH=C(CH_3)CH_3$

2. Draw the following compounds:

methylbutane; cyclopentane; but-1-yne; 3-ethylpent-1-ene; 3-chlorobut-1-ene; 1,1-dichloropropane; 2,2,4-trimethylheptane; pent-2-yne; propan-1,2-diol; 2-methylbutan-2-ol

6) Homologous series

Organic compounds with the same functional group, but a different number of carbon atoms, are said to belong to the same **homologous series**. Every time a carbon atom is added to the chain, two hydrogen atoms are also added.

A homologous series is a series of organic compounds which have the same functional group, but in which the formula of each successive member increases by -CH_2-.

Eg Homologous series of unbranched alkanes:
CH_4, CH_3CH_3, $CH_3CH_2CH_3$, $CH_3CH_2CH_2CH_3$, $CH_3(CH_2)_3CH_3$, $CH_3(CH_2)_4CH_3$ etc

Eg Homologous series of alcohols:
CH_3OH, CH_3CH_2OH, $CH_3CH_2CH_2OH$ etc

As a homologous series is ascended, the size of the molecule increases. Therefore the Van der Waal’s forces between the molecules become stronger and the boiling point increases.

7) Isomerism

Isomers are molecules which have the same molecular formula but different structures.

There are a number of different types of isomerism in organic compounds, which can be classified as **structural isomerism** or **stereoisomerism**.

a) Structural Isomerism

Structural isomers are molecules which have the same molecular formula but a different arrangement of covalent bonds.

The different arrangement of covalent bonds can result from:

i) The functional group being in different positions (**positional isomerism**)
ii) A different arrangement of the carbon skeleton (**chain isomerism**)
iii) A different functional group (**functional isomerism**)

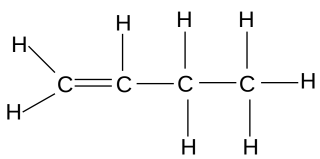
i) Positional isomerism

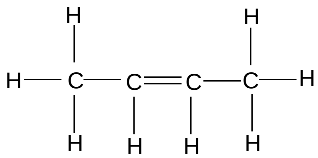
Positional isomers are molecules with the same molecular formula but which have the functional group on different positions in the molecule.

Alkanes do not show functional isomerism as they have no functional group.

Alkenes with four or more carbon atoms show positional isomerism:

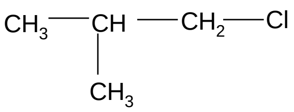
Eg but-1-ene and but-2-ene

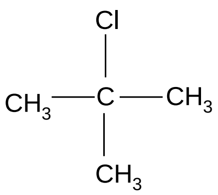




Halogenoalkanes and alcohols with three or more carbon atoms show positional isomerism

Eg 1-chloromethylpropane and 2-chloromethylpropane



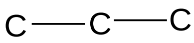


ii) **Chain isomerism**

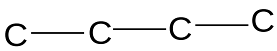
Chain isomers are molecules with the same molecular formula but a different arrangement of carbon atoms.

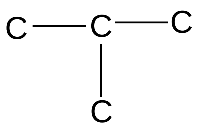
The arrangement of carbon atoms in an organic molecule is known as the carbon skeleton.

Carbon skeletons containing up to three carbon atoms can only be arranged in one way – i.e. a straight chain with no branching:

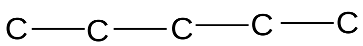


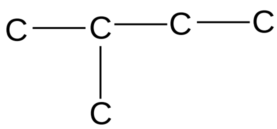
Carbon skeletons containing four carbon atoms can be arranged in two ways:

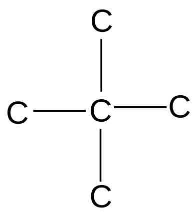




Carbon skeletons containing five carbon atoms can be arranged in three ways:

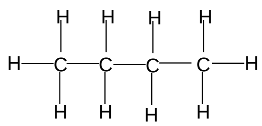


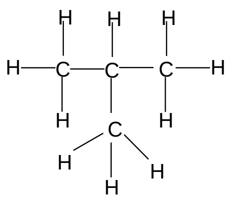




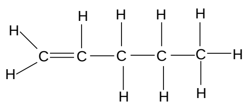
All molecules containing four or more carbon atoms can thus show chain isomerism:

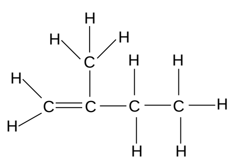
Eg butane and methylpropane



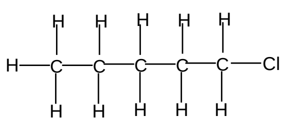


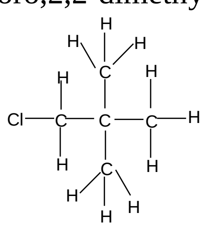
Eg pent-1-ene and 2-methylbut-1-ene





Eg 1-chloropentane and 1-chloro,2,2-dimethylpropane



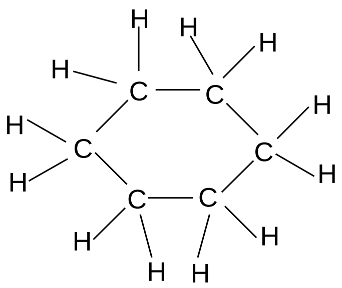


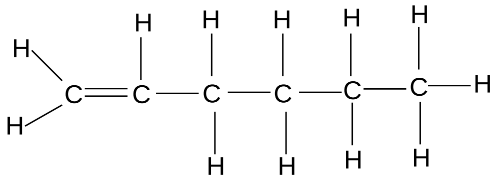
iii) **Functional isomerism**

Functional isomers are molecules with the same molecular formula but different functional groups.

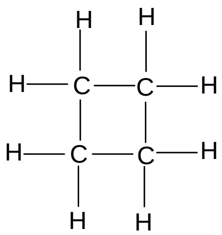
eg Alkanes which have a ring rather than a straight chain arrangement are known as cycloalkanes. They have the general formula C_nH_{2n}, which is the same as alkenes. Cycloalkanes and alkenes can thus show functional isomerism.

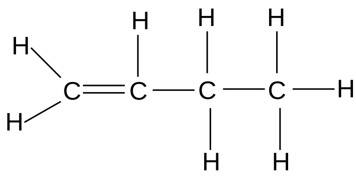
Eg cyclohexane and hex-1-ene





Eg cyclobutane and but-1-ene



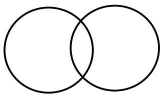


b) Stereoisomerism

It is possible for a two molecules to have the same atoms bonded to each other but to be different due to a different spatial arrangement. This is known as stereoisomerism. The only type of stereoisomerism required for WASSCE Chemistry is **geometrical isomerism**.

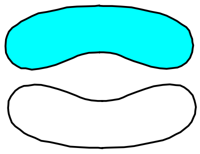
Stereoisomers are molecules with the same structural formula but a different spatial arrangement of atoms.

In double bonds, the first bond involves an overlap of atomic orbitals directly in between the nuclei of the two atoms:



This is known as a σ-bond. All single covalent bonds are σ-bonds.

The second bond, however, cannot bond in the same place. Instead, two p-orbitals overlap above and below the internuclear axis:



This is known as a π-bond. All double covalent bonds consist of one σ-bond and one π-bond.

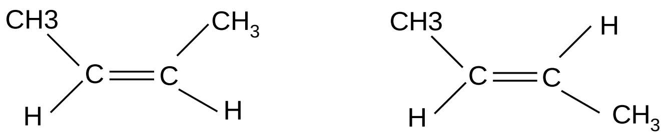
Since these orbitals overlap in two places, it is not possible to rotate a π-bond about its axis without breaking the bonds. There is thus restricted rotation about the double bond. If both carbon atoms on either side of the bond are attached to different groups, then two different structures arise which cannot be interconverted. This is known as geometrical isomerism.

Geometrical isomers are stereoisomers with different spatial orientations around the carbon-carbon double bond.

It is caused by the restricted rotation about a carbon-carbon double bond.

It arises when the carbon atoms on both sides of the bond are attached two different groups.

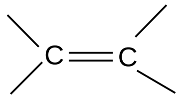
Eg but-2-ene has two geometrical isomers:



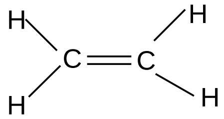
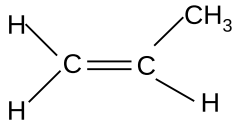
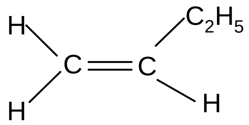
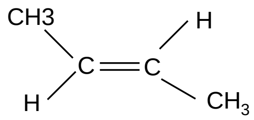
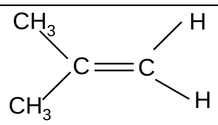
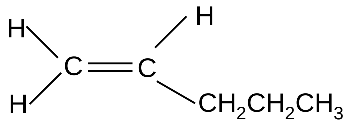
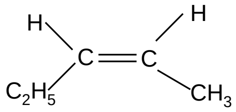
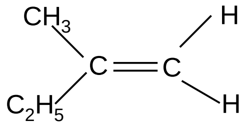
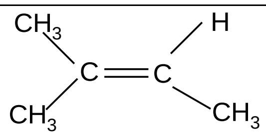
These two isomers cannot be interconverted without breaking the π-bond.

Note that molecules which show geometrical isomerism always have two specific structural features:
- there is a carbon-carbon double bond
- both the carbon atoms are attached to two different groups.

Geometrical isomers should always be drawn using **crab notation**. Crab notation shows the C=C bond as a planar centre with the 4 groups shown as follows:



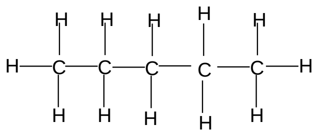
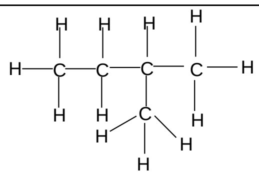
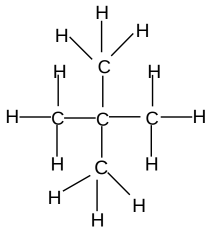
Using crab notation, it is easy to predict whether geometrical isomerism will exist in molecules.

Ethene		No geometrical isomerism
Propene		No geometrical isomerism
But-1-ene		No geometrical isomerism
But-2-ene		Geometrical isomerism
2-methylpropene		No geometrical isomerism
Pent-1-ene		No geometrical isomerism
Pent-2-ene		Geometrical isomerism
2-methylbut-1-ene		No geometrical isomerism
2-methylbut-2-ene		No geometrical isomerism

c) Distinguishing between isomers

Isomers tend to differ slightly in their melting and boiling points. Molecules with no branching tend to have higher boiling points than isomers with more branching. This is because they have a higher surface area, so they pack together better and so the van der Waal's forces are stronger.

Eg isomers of pentane, C_5H_{12}:

Isomer	Structure	Boiling point/^oC
Pentane		36
Methylbutane		28
2,2-dimethylpropane		10

Test Your Progress: Unit 7 Part 1 Exercise 3

1. Draw the four structural isomers of $C_4H_{10}O$ and name them.

2. Molecules A, B, C, D, E and F are all isomers with the molecular formula C_4H_8. A and B are alicyclic. C is a branched alkene. D is an unbranched alkene. E and F are geometrical isomers of each other. Draw and name all six molecules.

3. How many structural isomers exist with the molecular formula $C_3H_6Cl_2$?