# ANDERSON SERANGOON JUNIOR COLLEGE JC1 H2 CHEMISTRY INTRODUCTION TO ORGANIC CHEMISTRY

#### Important note:

The Learning Outcomes (LOs) that are greyed out will be covered in subsequent Organic Chemistry chapters.

#### Contents

Empirical, molecular and structural formulae Functional groups and the naming of organic compounds Common terms for organic reactions and reactivities Shapes of organic molecules;  $\sigma$  and  $\pi$  bonds

#### Learning Outcomes (LOs)

Candidates should be able to:

- (a) interpret, and use the nomenclature, general formulae and displayed formulae of the following classes of compound:
  - (i) hydrocarbons (alkanes, alkenes and arenes)
  - (ii) halogen derivatives (halogenoalkanes and halogenoarenes)
  - (iii) hydroxyl compounds (alcohols and phenols)
  - (iv) carbonyl compounds (aldehydes and ketones)
  - (v) carboxylic acids and derivatives (acyl chlorides and esters)
  - (vi) nitrogen compounds (amines, amides, amino acids and nitriles)
- (b) interpret, and use the following terminology associated with organic reactions:
  - (i) functional group
    - (ii) degree of substitution: primary, secondary, tertiary and quaternary
    - (iii) homolytic and heterolytic fission
    - (iv) carbocation
    - (v) free radical, initiation, propagation, termination
    - (vi) electrophile (Lewis acid), nucleophile (Lewis base)
    - (v) addition, substitution, elimination, condensation, hydrolysis
    - (vi) oxidation and reduction
      - [in equations for organic redox reactions, the symbols [O] and [H] are acceptable]
- (c) interpret, and use the following terminology associated with organic reactivities:
- (i) delocalisation
  - (ii) electronic effect (electron-donating and electron-withdrawing effect)
  - (iii) steric effect (steric hindrance)
- (d) describe sp<sup>3</sup> hybridisation, as in ethane molecule, sp<sup>2</sup> hybridisation, as in ethene and benzene molecules, and sp hybridisation, as in ethyne molecule
- (e) explain the shapes of, and bond angles in, the ethane, ethene, benzene, and ethyne molecules in relation to  $\sigma$  and  $\pi$  carbon–carbon bonds
- (f) predict the shapes of, and bond angles in, molecules analogous to those specified in (e)
- (g) apply (b) and (c) to the understanding of mechanisms in terms of organic structure and bonding
- (h) recognise that the mechanism of polar reactions involve the flow of electrons from electron-rich to electron-poor sites

#### References

- 1. Chemistry for Advanced Level, Cann and Hughes, Murray
- 2. Organic Chemistry, McMurry, Brooks/ Cole
- 3. Understanding Advanced Physical Inorganic Chemistry, Jeanne Tan and Kim Seng Chan

#### I. INTRODUCTION

Organic chemistry is the branch of chemistry concerned with the study of compounds containing carbon. This includes the vast majority of carbon-containing compounds, except for compounds such as CO,  $CO_2$  and carbonates that are traditionally considered to belong to the field of inorganic chemistry.

Every living organism is made of organic chemicals. The proteins that make up our hair, skin and muscles; the DNA that controls our genetic heritage; the food that nourish us; the clothes that keep us warm; and the medicines that heal us are mainly organic chemicals.

Today, organic chemicals outnumber inorganic ones by 80:1, and number well over 10 million different compounds. The large variety of organic compounds arises due to 2 main reasons:

1. Carbon atoms can form strong bonds with other carbon atoms. Such bonding allows chains and rings of carbon atoms of various lengths to be produced.

Example: the 4 different ways to arrange 4 linked carbon atoms

$$C-C-C-C$$
  $C$   $C-C-C$   $C-C$   $C-C^-C$ 

Moreover, each carbon atom can form <u>four bonds</u>. This allows branched chains, multiple bonds and attachment of other atoms to occur, further increasing the number of structures possible.

4 single	2 single and	2 double bonds	1 single and
covalent bonds	1 double bond		1 triple bond
C	C==	—C—	—C≡

2. Generally organic compounds are <u>kinetically</u> stable. Many organic reactions possess a <u>high activation energy</u> which must be supplied before the reaction will proceed. This is a result of the strong covalent bonds formed. These bonds have to be broken before reaction can occur, and breaking strong bonds require much energy.

If the right conditions and catalysts can be found, it is possible to convert one organic compound into another.

In subsequent topics, we will look at the reactions and properties of a number of organic compounds.

#### **II. GENERAL PROPERTIES OF ORGANIC COMPOUNDS**

(a) Melting point and Boiling point

Organic molecules generally have <u>low melting points and boiling points</u>. They are held by <u>weak intermolecular forces of attraction</u> (i.d.–i.d., p.d.–p.d. or hydrogen bonds) which can be overcome easily by heating.

(b) Solubility

<u>Low solubility or insoluble</u> in polar solvents (e.g. water) except when polar groups such as -OH, -COOH and  $-NH_2$  are present in the molecule.

Most organic compounds are only soluble in <u>non-polar organic solvents</u>, such as benzene and ether.

(c) Thermal stability

Organic compounds are usually <u>thermally unstable</u>, decomposing into smaller molecules when heated to temperatures above 500 °C.

Example, when heated, butane-1,4-dioic acid decomposes as follows:



(d) Flammability

Many organic compounds are <u>flammable</u> and <u>burn exothermically</u> in a plentiful supply of air to yield carbon dioxide and water. Thus most fuels are organic compounds (e.g. oil, petrol and natural gas), and their combustion is our main source of heat energy.

e.g.  $C_2H_5OH + 3O_2 \longrightarrow 2CO_2 + 3H_2O$ 

(e) Reactivity

Rate of organic reactions are <u>usually slow</u> compared to inorganic reactions. They usually require <u>heating</u> or the use of a <u>catalyst</u> to speed up reactions in the laboratory or in the industry. This is due to the high activation energy to break strong covalent bonds.

For example, concentrated H<sub>2</sub>SO<sub>4</sub> is used as a catalyst in the esterification reaction.

$$H_3C-CH_2-OH + H_3C-COH COH CONC. H_2SO_4 H_3C-C-O-CH_2-CH_3 + H_2O$$

#### **III. HYBRIDISATION IN ORGANIC COMPOUNDS**

Covalent bonds are formed when atomic orbitals overlap. However, when one tries to derive the shape of a molecule using the overlap of atomic orbitals, sometimes its geometry does not correspond to the geometry as predicted by the VSEPR model (which is observed experimentally). For instance, in CH<sub>4</sub>, if all the bonds on CH<sub>4</sub> are formed using s and p orbitals in C atom, since the three 2p orbitals that carbon used in bond formation are perpendicular to each other, wouldn't three of the four C-H bonds be 90° to each other? Why is there a tetrahedral arrangement of the four C-H bonds and all the bond angles 109.5° instead?

Hybridisation is a solution that reconciles the overlap of atomic orbitals with the VSEPR model to explain what is observed experimentally. It is essentially the mathematical mixing of atomic orbitals to create new orbitals (known as hybrid orbitals) which are used to form <u>sigma bonds</u> in bonding. (This will be illustrated in the examples on pages 5 to 10)

Combinations of different numbers of atomic orbitals give rise to different types of hybrid orbitals.

The hybrid orbitals take up a distinctive shape and relative orientation, depending on the number and type of atomic orbitals that have been mixed. The total number of atomic orbitals on an atom remains constant, and so the <u>number of hybrid orbitals</u> on an atom <u>equals</u> the <u>number of atomic orbitals mixed</u>.

In organic chemistry, our focus is hybridisation in molecules containing the <u>carbon</u> atom, although hybridisation can also be applied to molecules containing other atoms.

The first step in constructing the hybrid orbitals is the process of **excitation** where a 2s electron is promoted to a vacant 2p orbital of higher energy.



The **3 types** of hybridisation (**sp**<sup>3</sup>, **sp**<sup>2</sup>, **sp**) will be illustrated using different compounds as examples.

	Type of hybridisation	sation Example	
(a)	sp³	ethane, $C_2H_6$ and methane $CH_4$	
(b)	sp²	ethene, C <sub>2</sub> H <sub>4</sub>	
(c)	sp	ethyne, C <sub>2</sub> H <sub>2</sub>	

## (a) <u>sp<sup>3</sup> hybridisation</u>

#### Example 1: Methane, CH<sub>4</sub>

For the carbon atom in methane, four valence orbitals (one 2s and three 2p orbitals) are mixed and four identical hybrid orbitals (called sp<sup>3</sup> hybrid orbitals) are formed.



Each hybrid orbital will have the same energy, which will be intermediate between the energies of the 2s and 2p orbitals.



- Four sp<sup>3</sup> hybrid orbitals of carbon overlaps head–on with four 1s hydrogen orbitals
- Carbon forms four C–H σ bonds with four adjacent H atoms.
- Hence, the molecule is tetrahedral with bond angles of 109.5°



# Example 2: Ethane, C<sub>2</sub>H<sub>6</sub>

In **each** of the two carbon atoms, four valence orbitals (one 2s and three 2p orbitals) are mixed and four identical hybrid orbitals (called sp<sup>3</sup> hybrid orbitals) are formed.





# (b) <u>sp<sup>2</sup> hybridisation</u>

## Example: Ethene, C<sub>2</sub>H<sub>4</sub>

In each of the two carbon atoms, three orbitals (one 2s and two 2p orbitals) are mixed and three identical hybrid orbitals (called sp<sup>2</sup> hybrid orbitals) are formed.



Note that each single bond is made up of one  $\sigma$  **bond**.

The two parallel unhybridised 2p orbitals from the two carbon atoms overlap side–on (p-p overlap) to give a  $\pi$  bond:



A double bond is hence described as  $1 \sigma$  bond and  $1 \pi$  bond.



For each carbon atom,

- Two sp<sup>2</sup> hybrid orbitals of carbon overlap head–on with two 1s hydrogen orbital, forming 2 C–H σ bonds
- **1 remaining** sp<sup>2</sup> hybrid orbital overlaps head-on with the sp<sup>2</sup> hybrid orbital of the neighbouring carbon atom to form the C–C  $\sigma$  bond
- The **unhybridised** p–orbital on each carbon aligns in such a way that it overlaps side–on with the p-orbital of the other carbon atom to form a π bond.
- Hence, the carbon–carbon **double bond** is made up of **1 strong \sigma–bond** and **1 weaker**  $\pi$ –bond
- The molecule is trigonal planar about each C atom with a bond angle of **120**°.

# Example: Benzene, C<sub>6</sub>H<sub>6</sub>

(More details will be given in the topic of "Arenes".)

Structure of benzene

In each of the six carbon atoms (each point of the hexagon represents a carbon atom), three orbitals (one 2s and two 2p orbitals) are mixed and three identical hybrid orbitals (called  $sp^2$  hybrid orbitals) are formed.

# (c) <u>sp hybridisation</u>

# Example: Ethyne, C<sub>2</sub>H<sub>2</sub>

In each of the two carbon atoms, two orbitals (a 2s and a 2p orbital) are mixed and two identical hybrid orbitals (called sp hybrid orbitals) are formed.



Both pairs of parallel unhybridised 2p orbitals overlap (**p-p overlap**) to give two  $\pi$  bonds.

E.g. : In the diagram above, to form  $\pi(1)$ , both C atom uses the unhybridised p orbital in the vertical plane to overlap sideway, above and below the sigma bond.

The triple bond between the two carbon atoms is thus made up of  $\frac{1 \sigma}{\sigma}$  bond and  $2 \pi$  bonds.

#### In summary: C<sub>2</sub>H<sub>2</sub> (ethyne)

- **One sp** hybrid orbital of carbon overlap head–on with the one 1s hydrogen orbital to form 1 C–H  $\sigma$  bond
- The other sp hybrid orbital overlap head-on with the neighbouring sp hybrid orbital of another carbon atom to form the C–C  $\sigma$  bond
- The **two unhybridised p** orbitals on each carbon aligns in such a way that overlaps side—on to form two  $\pi$  bonds (see  $\pi(1)$  and  $\pi(2)$  bonds in the diagram below).
- Hence, the carbon–carbon triple bond is made up of one strong  $\sigma$ –bond and two weaker  $\pi$ –bonds.
- Hence, ethyne is **linear** about each carbon with bond angle of **180**<sup>0</sup>.



#### Checkpoint 1

How many  $\sigma$  and  $\pi$  bonds are there in a molecule of the following compound?

	<u>σ</u>	<u>π</u>
Α	5	4
В	7	2
С	8	1
D	15	2

Solution:



There are <u>single</u> and <u>double</u> bonds.

Each single bond is made up of 1  $\sigma$  bond. Each double bond is made up of 1  $\sigma$  bond and 1  $\pi$  bond.

Total no. of  $\sigma$  bonds = \_\_\_\_\_ Total no. of  $\pi$  bonds = \_\_\_\_\_ In short, to determine the hybridisation state of an atom, we can also make use of the following guidelines:

number and type of bonds around atom	number of electron regions (bond pairs + lone pairs)	^Shape about hybridised C w.r.t number of electron regions	atomic orbitals undergoing hybridisation	(valence) atomic orbitals unhybridised	type of hybrid orbital formed / hybridisation state of atom	Bond angle	* % of s character in hybrid orbital
4 single bonds							
H E.g.	4	Tetrahedral	s, p, p, p	_	sp³	109.5°	25.0
2 single bonds and 1 double bond <u>OR</u> 3 $\sigma$ bonds and 1 $\pi$ bond H E.g.	3	Trigonal planar	s, p, p	p	sp²	120°	33.3
1 single bond and 1 triple bond <u>OR</u> 2 $\sigma$ bonds and 2 $\pi$ bonds E.g. H-C=C-H	2	Linear	s, p	p, p	sp	180°	50.0

# Note:

A The hybridisation state of the carbon atom can be deduced from the shape about the C w.r.t number of electron regions (and vice versa).
 \* % s character is calculated based on relative contribution of s orbital in hybrid orbital. E.g. sp<sup>3</sup> hybrid orbitals is made up of one s orbital and three p orbitals. hence, one s orbital out of four orbitals in total is 25% s character. More details can be found on page 14.

# Checkpoint 2

What is the number of  $sp^2$  hybridised carbon atoms present in the organic molecule **Y** as shown below?



Number of sp<sup>2</sup> hybridised carbon:

#### Note

The 2s and 2p orbitals of O and N atoms in molecule  $\mathbf{Y}$  above can hybridise in the same way as the 2s and 2p orbitals of C atoms.

Here's the hybridisation state of O and N atoms in the above example.

Atom	number of electron regions (bond pairs + lone pairs)	Shape about the atom w.r.t number of electron regions	Hybridisation state
0	3	Trigonal planar	sp <sup>2</sup>
Ν	2	Linear	sp

#### Effect of hybridisation on covalent bond strengths

One of the factors affecting bond strength is the hybridisation state of bonding atom.

• Hybrid orbitals are formed on mixing atomic orbitals of the same atom. Hence, a hybrid orbital formed on mixing the s orbital and p orbitals has partial s and p character.

Hybrid	% character in hybrid orbital	
orbital	s	p
sp³	25	75
sp²	33	67
sp	50	50

# Recall in Chemical Bonding: Why are C-C bonds in graphite stronger than those in diamond?

- Carbon in graphite is sp<sup>2</sup> hybridised while the one in diamond is sp<sup>3</sup> hybridised.
- Greater s character in the hybrid orbital used to form bond will lead to:
- more effective overlap of the orbitals when forming bonds
  - stronger bond formed
  - shorter bond length
- Reason: <u>Electrons in s orbitals</u> are held <u>more closely to the nucleus</u> than <u>electrons in p</u> <u>orbitals</u>. Hence, hybrid orbital that has <u>more s character</u> will have its <u>electrons</u> <u>held more closely</u> to the nucleus and more strongly attracted to it, compared to one that has less s character.

#### Checkpoint 3 (N2008/I/19)

The bond lengths in buta-1,3-diene differ from those which might be expected.

The carbon-carbon bond length in ethane is 0.154 nm and in ethene 0.134 nm. The central single bond in buta-1,3-diene (C2-C3), however, is shorter than the single bond in ethane: it is 0.147 nm.



Which helps to explain this C2-C3 bond length?

- **A** It is an  $sp^2 sp^2$  overlap.
- **B** It is an  $sp^2$ — $sp^3$  overlap.
- **C** The electrons in the filled *p* orbitals on C2 and C3 repel each other.
- **D** The  $sp^3$ — $sp^3$  bonding is pulled shorter by a p— $p(\pi$  bond) overlap.

Answer:

#### Reason:

Both C2 and C3 have	hybridised orbitals which have	
character resulting in	effective overlap than the	overlap in
ethane molecule.		

#### **IV. CLASSIFICATION OF ORGANIC COMPOUNDS**

The simplest organic compounds are **hydrocarbons**, compounds containing only carbon and hydrogen. All other organic compounds (e.g. containing O, N, and halogen atoms) are derivatives of hydrocarbons.

- **1. Saturated** hydrocarbons are hydrocarbons that contain only single bonds between the atoms.
- 2. Unsaturated hydrocarbons are hydrocarbons that contain double or triple bonds between atoms.
- **3.** Aromatic hydrocarbons are hydrocarbons that contain at least one benzene ring. (We will discuss aromatic compounds in Arenes chapter.)

CH<sub>3</sub>





Benzene

phenol

- 4. Non-aromatic hydrocarbons are often referred to as **aliphatic** hydrocarbons.
- **5.** A **cyclic** (or alicyclic) hydrocarbon is one in which a chain of carbon atoms has formed a ring.

methylbenzene



Many organic compounds consist of a hydrocarbon chain with one or more reactive groups attached. These <u>reactive groups</u> responsible for a <u>characteristic chemical behaviour</u> are called **functional groups**.

Each functional group has characteristic reactions, and are relatively unaffected by the size and shape of the hydrocarbon skeleton it is attached to. The characteristic reactions of the different functional groups will be covered in detail in subsequent topics.

For a compound containing more than one functional group, its properties as a whole can be predicted by considering the effect of each functional group present in the molecule.

Common functional groups:

Name of homologous series	Functional group	General formula	Example
Alkane	C-C	$C_nH_{2n+2}$	$CH_4, C_2H_6$
Alkene	)_C=C	$C_nH_{2n}$	$CH_2=CH_2$
Arene		Ar —	
Halogenoalkane	— X (F, C <i>l</i> , Br or I)	R — X	CH₃CH₂Br
Alcohol	— OH	R — OH	CH₃CH₂OH

Aldehyde	О —С—Н	O ∥ R—C—H	CH₃CHO
Ketone	O C	0    R—C—R'	$\overset{O}{\overset{\parallel}{\overset{\parallel}{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle\sqcup}}{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle\sqcup}}{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle }{\overset{\scriptstyle\sqcup}{\overset{\scriptstyle }{\overset{\scriptstyle }}{\overset{\scriptstyle }{\overset{\scriptstyle }{\overset{\scriptstyle }}{\overset{\scriptstyle }}}{\overset{\scriptstyle }}{\overset{\scriptstyle }}{\overset{\scriptstyle }}{\overset{\scriptstyle }}{\overset{\scriptstyle }}{\overset{\scriptstyle }}}{\overset{\scriptstyle }}{\overset{\scriptstyle }}}}}}}}}}$
Carboxylic acid	О — — С—ОН	O II R—C—OH	CH <sub>3</sub> CO <sub>2</sub> H
Acid chloride	O —C —C CI	O ⊫ R—C—CI	CH₃COCI
Ester	0 — C—O—	0    R—C—O—R'	$CH_3 - C - O - CH_2CH_3$
Amine	— NH <sub>2</sub>	$R - NH_2$	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>
Amide	0 —C—N—	O 	CH <sub>3</sub> CONH <sub>2</sub>
Amino acid	H <sub>2</sub> N—C—COOH	R H <sub>2</sub> N—C—COOH R'	H <sub>2</sub> N-CH <sub>2</sub> -COOH
Nitriles	—C≡N	R─C≡N	CH <sub>3</sub> CH <sub>2</sub> CN

\* R denotes the rest of the molecule

A homologous series is a series of organic compounds, with the same functional group, varying only in the length of the carbon chain.

Homologues are successive members of the series, with similar chemical properties since they contain the same functional group.

The molecular formulae of members of the series fit the same general formula. For adjacent members of the series, their molecular formulae differ by a fixed group of atoms.

While the length of carbon chain has little effect on the chemical reactivity of the functional group, it does affect physical properties (such as solubility, melting point and boiling point). Thus the physical properties change throughout the series in a regular way.

Name	Formula	Boiling point / °C
Methane	$CH_4$	-164
Ethane	CH <sub>3</sub> CH <sub>3</sub>	-89
Propane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	-42
Butane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	0

e.a. (	straight-chain alkanes)	):
- g. v		<i>.</i>

		A
)	Recall from	
	'Chemical	
	Bonding' to	
	explain this	
	trend.	

## V. IUPAC NOMENCLATURE OF ORGANIC COMPOUNDS

Chemists throughout the world use the International Union of Pure and Applied Chemistry (IUPAC) as a systematic form of nomenclature for organic compounds. Each name can consist of the components listed below.

Prefix(es) – Parent – Suffix

1. Parent – specifies the number of carbon atoms in the longest carbon chain.

Parent	meth-	eth-	prop-	but-	pent-	hex-	hept-	oct-	non–	dec-
No. of C atoms	1	2	3	4	5	6	7	8	9	10

If the carbon atoms are joined in an aliphatic ring, the prefix 'cyclo' is added.

e.g.

Name	propane	cyclobutane
Structural formula	CH3CH2CH3	H H H-C-C-H H-C-C-H H-C-C-H H H

2. Suffix – indicates the principal functional group present in the compound.

Suffix	Meaning		Suffix	Meaning
-ane	all C-C single bonds		-ol	alcohol (—OH group)
-ene	1 C=C double bond		-al	aldehyde (—CHO group)
-diene	2 C=C double bonds		-one	ketone (—CO— group)
-triene	3 C-C double bonds	double bonds	-oic acid	carboxylic acid group
				(—CO <sub>2</sub> H)

Where there are more than one of the same principal functional group present in the molecule, prefixes 'di' and 'tri' are used to indicate the number of the same principal functional group present. The positions of the functional groups are indicated by Arabic numerals.

e.	a	
	Э	•

Name	Structural formula	
but-2-ene	CH₃CH=CHCH₃	
penta-1,3- <b>di</b> ene	CH <sub>2</sub> =CHCH=CHCH <sub>3</sub>	
propane-1,2- <b>di</b> ol	$\begin{array}{ccc} OH & OH \\   &   \\ CH_2 - CH - CH_3 \end{array}$	

Note that in naming organic compounds:

- a <u>number</u> and a <u>letter</u> are separated by a <u>hyphen '-'</u>
- <u>two numbers</u> are separated by a <u>comma ','</u>

3	Prefix _	indicates	substituent	aroun(s)	on the i	narent
J.	FIEIX -	· IIIuicales	SUDSLILUEIIL	group(s)		Jaieni.

Prefix	Meaning	Prefix	Meaning
methyl	CH3-	fluoro	-F
ethyl	CH <sub>3</sub> CH <sub>2</sub> -	chloro	-C <i>l</i>
propyl	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> -	bromo	-Br
phenyl	C <sub>6</sub> H <sub>5</sub> -	iodo	-I
nitro	-NO <sub>2</sub>	hydroxy	-OH

Prefixes can be combined and they might in turn be prefixed to show multiple substitution.

Prefixes:

di = 2	tri = 3	tetra = 4	penta = 5	hexa = 6
hepta = 7	octa = 8	nona = 9	deca = 10	

The *position of a substituent group* along the carbon chain is indicated by an <u>Arabic numeral before the substituent</u>.

In our syllabus, the focus is not on naming a compound. Rather, it is being <u>able to work from</u> <u>the name to the correct structural formula</u>.

To work out the correct structural formula from the name, it is often easier to work backwards from the 'parent' hydrocarbon.

# Checkpoint 4

Name	Structural formula
1,2-dimethylcyclohexane	
3-chloropropanal	
3-methylbut-2-en-1-ol	

If there are more than one substituent group, they are arranged in alphabetical order. (E.g. <u>c</u>hloro before <u>m</u>ethyl)

# <u>Checkpoint 5</u>

Name	Structural formula
2-chloro-3-methylbutane (not 3-methyl-2-chlorobutane)	

The carbon atoms in the longest carbon chain are numbered successively from the end that results in the smallest overall numbers.

# Checkpoint 6

Name	Structural formula
1,2-dichloropropane (not 2,3-dichloropropane)	

## VI. Types of representation

Many organic compounds are more complex structurally than inorganic compounds. Several different types of formulae can be used to represent organic compounds, depending on the amount of information required.

- Empirical formula shows which elements are present in the compound, and the simplest ratio of the number of atoms of the elements present in one molecule.
   e.g. CH<sub>2</sub>O
- 2. **Molecular formula** a multiple of the empirical formula; shows the <u>actual number of atoms of each element present in one molecule</u>. e.g.  $C_3H_6O_3$
- Structural formula shows <u>how constituent atoms of a molecule are joined together in a molecule</u>. Can be *condensed*, *displayed*, *skeletal* or *stereochemical*.
   e.g. CH<sub>3</sub>CH(OH)CO<sub>2</sub>H

When answering questions, you need to show clearly how the groups of atoms are positioned in the molecule for an unambiguous structure, e.g.  $CH_3CH_2CH_2OH$  for propan-1-ol, not  $C_3H_7OH$ .

(i) **Condensed formula** – each carbon atom is written separately, along with the atoms or groups attached to it. The <u>bonds around each carbon atom are not explicitly shown</u>.

<u>C=C double bonds are shown in condensed formulae</u>, where this makes the structure clearer. <u>Branches in the carbon chains are indicated in brackets</u>.

e.g.

Structure	H_C=C <h_h< th=""><th><math display="block">\begin{array}{c} H\\ CH_3 \longrightarrow CH_3\\ CH_3 \end{array}</math></th></h_h<>	$\begin{array}{c} H\\ CH_3 \longrightarrow CH_3\\ CH_3 \end{array}$
Condensed formula	CH <sub>2</sub> =CH <sub>2</sub>	CH <sub>3</sub> CH(CH <sub>3</sub> )CH <sub>3</sub>

(ii) Full structural or Displayed formula – <u>detailed structure</u> of molecule showing the relative placing of atoms and the number of bonds between them (single / double / triple).



(iii) Skeletal formula – <u>simplified representation</u> of an organic formula derived from the structural formula by removing hydrogen atoms (and their associated bonds) and carbon atoms from alkyl chains, <u>leaving just the carbon–carbon bonds in the carbon skeleton and</u>

the associated functional groups. This is a useful way of describing large and complicated molecules.

Skeletal or partial skeletal representations may be used in question papers and can be acceptable in answers where they are unambiguous.



Straight lines representing carbon–carbon bonds are <u>drawn in a zigzag format</u>, where the <u>end of every line represents a carbon atom</u>. <u>C–H bonds are not shown in a skeletal</u> <u>formula</u>. Each carbon is assumed to form enough C–H bonds to make a total of 4 bonds, unless shown otherwise.

Carbon rings are often represented by their skeletal formula.



(iv) Stereochemical formula – shows <u>spatial arrangement</u> of bonds, atoms and groups in molecule in 3-dimensional. Usually only used when it is important to show the shape of a molecule.



*Checkpoint* 7 (different types of formula to represent ethanoic acid)

Empirical	Molecular	Structural			
		Condensed	Displayed	Skeletal	Stereochemical

#### VII. Types of reaction

Organic reactions can be classified under a few broad types of reactions based on structural changes in *reactant molecules*.

Addition – occurs when two reactants 'add' together to form a single new product. It
usually involves a reagent adding across an unsaturated bond of a compound to produce
a single product.

e.g.



- Elimination occurs when <u>a pair of atoms</u> or <u>groups of atoms</u> are <u>removed</u> from a <u>single</u> molecule (you may imagine it as a single reactant 'splits' into two products). It usually involves the <u>removal of atoms or groups of atoms</u> that are <u>adjacent to each other</u> to form <u>a multiple bond</u> (i.e. double or triple bond).
  - e.g.



3. **Substitution** – occurs when <u>one atom or groups of atoms</u> in a compound is <u>replaced by</u> <u>another atom or groups of atoms</u>.

e.g.



 Hydrolysis – occurs when <u>covalent bond</u> in an organic molecule is <u>broken</u> after reaction with <u>water</u>. You may imagine it as a reactant is 'split' into two products by the action of water (<u>often in the presence of OH<sup>-</sup> or H<sup>+</sup> as catalysts</u>).

e.g.

$$\begin{array}{c} O & O \\ \parallel \\ CH_3 - C - Cl + H_2O \longrightarrow CH_3 - C - OH + HCl \end{array}$$

5. **Condensation** (or addition–elimination) – occurs when <u>two reactants react to form a single</u> <u>product</u>, <u>with the elimination of a small molecule</u> (such as water or HC*l*).

e.g.

$$CH_{3} - CH_{3} + H - N - R - P CH_{3} - CH_{3} + H - N - R + H_{2}O$$

#### 6. Redox reactions in organic compounds

 (i) Oxidation – a reaction in which the <u>oxidation number</u> of the reactive carbon/atom in the functional group <u>increases</u>.

e.g.  $CH_3CH_2OH + 2[O] \longrightarrow CH_3COOH + H_2O$ 

 (ii) Reduction – a reaction in which the <u>oxidation number</u> of the reactive carbon/atom in the functional group <u>decreases</u>.

e.g.  $CH_3CN + 4[H] \longrightarrow CH_3CH_2NH_2$ 

In equations for organic redox reactions, the symbols [O] and [H] are acceptable.

\_\_\_\_\_

#### (iii) Determination of Oxidation number of elements in organic species

Unlike metals, which are almost always in a positive oxidation state, the oxidation state of carbon can vary widely in organic species.

When assigning oxidation numbers, the following rules apply:

- If <u>atoms of the same element</u> are bonded, 0 is assigned.
   e.g. For C=C, oxidation number of each C is 0.
- For bonds between atoms of different elements, assign -1 to the more electronegative atom for <u>each pair</u> of bonding electrons. The other atom is assigned +1.

e.g. C=OC-ON-H O-HC-H+1 -1 -1 +1 +2 -2 -1 +1 -1 +1 Reference: Electronegativities values of common elements in organic compounds. н С Ν Ο F 2.1 2.5 3.0 3.5 4.0 Ρ S CI 2.1 2.5 3.0 Br 2.8 Ι 2.5

# Checkpoint 8

Compound		Oxidation state of C	
methane CH₄	н, _н н, ⊂_, н н, ⊂, н		
ethane CH₃CH₃	H,, H H <sub>3</sub> C ⊂ _+H		
but-1-ene CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub>	H CH		
ethanoic acid CH₃CO₂H	H O  1   2 H—C—C—O—H   H	$\begin{array}{cccccccc} & +1 & -2 \\ & H & O \\ & +1 &   &   & -2 & +1 \\ & +1 & -C & -C & -O & -H \\ & & -3 &   & +3 \\ & & H \\ & & -3 &   & +3 \\ & & H \\ & & +1 \end{array} \qquad C2: \_$	



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## VIII. Applications

When you picked up your notes, your muscles were doing chemical reactions on sugars to give you the energy you needed. As you read these words now, your eyes are using an organic compound to convert visible light into nerve impulses and as you understand the notes, gaps between your brain cells are being bridged by simple organic molecules (neurotransmitter amines) so that nerve impulses can be passed around your brain. You did all that without consciously thinking about it! And all of these are related to organic chemistry!

Organic Chemistry is also known as the 'Chemistry of Life'. The clothes we wear, the plastics we use, the new drugs we take are all extension of organic chemistry. Here are some applications of organic chemistry in our daily lives.

#### Example 1: SUNSCREEN



We all know how harmful the UV rays can be to our skin. Over exposure to the sun can result in pre-mature aging, skin cancer wrinkles, severe burns and age spots. Excessive exposure may also impede the body's immune system. Protection from UV rays makes the use of sunscreen important.

The useful principal ingredients in sunscreens are usually <u>organic</u> aromatic molecules conjugated with carbonyl groups.

This general structure allows the molecule to absorb high–energy ultraviolet rays and release the energy as lower–energy rays, thereby preventing the skin–damaging ultraviolet rays from reaching the skin.

Some common organic molecules found in sunscreen are avobenzone, octyl salicylate and dioxybenzone.

# Example 2: ANTIBIOTICS



An antibiotic is any substance that interferes with the ability of bacteria to function normally. It may either inhibit their growth or kill the bacteria.

Antibiotics are used to treat bacterial infections but will not help cure illnesses caused by viruses, such as colds or flu.

Penicillin, the first antibiotic, was discovered in 1928 by Alexander Fleming in London, England. Fleming made his discovery when he noticed that bacteria could not survive on a culture plate that contained a mold commonly found on bread.



# **Structure of Penicillin**

Scientists spent the next few years learning to purify the penicillin from the mold. By the early 1940s, penicillin was widely available. Not long after, other antibiotics were discovered.

The discovery of penicillin was considered a medical miracle because it helped wiped out many of the diseases that are caused by bacteria. This meant that deadly diseases such as tuberculosis, pneumonia, syphilis and tetanus could now be treated.

#### Example 3: PLASTIC

Plastic is made up of **organic** compounds known as polymers, and are composed primarily of carbons, hydrogen and oxygen. Some physical properties of plastic include transparency, permeability, flexibility, elasticity, permeability and electrical resistance. Some chemical properties include low solubility in water, chemical resistance, moderate thermal stability, low reactivity with water and flammability.