1. Details of Module and its structure

Module Detail	
Subject Name	Chemistry
Course Name	Chemistry 01 (Class XI, Semester - 2)
Module Name/Title	Organic Chemistry – Some Basic Principles and Techniques: Part 1
Module Id	kech_21201
Pre-requisites	Knowledge about catenation, covalent bonding and hybridization
Objectives	After going through this lesson, the learners will be able to: • Differentiate between inorganic and organic compounds • Learn about various hybridization present in organic compounds • Explain various structural representations of organic compounds • Understand the classification of organic compounds
keywords	Structural Representations, 3d-Representation of Organic Molecules, Molecular Models, Open Chain Compounds, Closed Chain, Alicyclic Compounds, Aromatic Compounds and Functional Group

2. Development Team

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1. Introduction

In this module you will learn about the basic structure and classification of organic molecules. As you are aware that the element carbon has the unique property called catenation due to which it forms covalent bonds with other carbon atoms. It also forms covalent bonds with atoms of other elements like hydrogen, oxygen, nitrogen, sulphur, phosphorus and halogens. Thus, any compound whose molecules contain carbon and hydrogen is called organic compound. Organic compound includes hydrocarbons and derivatives of hydrocarbons. Organic compounds are studied under a separate branch of chemistry called organic chemistry.

For sustaining life on earth, organic compounds are vital and they include complex molecules like deoxyribonucleic acid (DNA) and proteins. DNA bears genetic information and proteins constitute essential compounds of our blood, muscles and skin. Some of the important areas of application of organic compounds are material like clothes, fuels, polymers, dyes and medicines. Science of organic chemistry is about two hundred years old. Although, the organic compounds are known to man since prehistoric times but their study practically started from the eighteenth century. Around the year 1780, chemists began to distinguish between organic compounds obtained from plants and animals and inorganic compounds prepared from mineral sources. In 1807, Berzilius, a Swedish chemist coined the term "organic compound" and he also proposed that a 'vital force' was responsible for the formation of organic compounds. However, this idea was rejected in 1828, when F. Wohler synthesised an organic compound, urea from an inorganic compound, ammonium cyanate.

$$\underset{\text{Ammonium cyanate}}{NH_4CNO} \xrightarrow{\text{Heat}} \underset{\text{Urea}}{NH_2CONH_2}$$

The synthesis of acetic acid by Kolbe (1845) and that of methane by Berthelot (1856) was revolution in field of synthetic organic chemistry and it was concluded that organic compounds could be synthesized from inorganic sources in a laboratory.

The development of electronic theory of covalent bonding ushered organic chemistry into its modern shape.

2. Tetravalency of Carbon

2.1 Hybridisation in carbon compounds

Carbon atom has $1s^2\ 2s^2\ 2p^2$ electronic configuration in ground state, however, in the excited state electronic configuration of carbon atom is $1s^2\ 2s^1\ 2p^1_x 2p^1_y 2p^1_z$. The 2s and 2p (Figure 1) orbitals of carbon atom are involved in hybridization. This leads to three types of hybridization which are *sp^3* (in alkanes), *sp^2* (in alkenes) and *sp* (in alkynes).

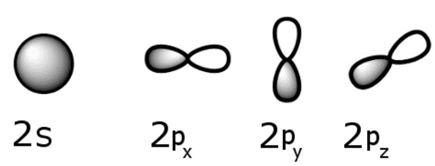


Figure 1

2.2 The Shapes of Carbon Compounds

The shapes of molecules like methane (CH_4), ethene (C_2H_4), ethyne (C_2H_2) are explained in terms of the use of sp^3, sp^2 and sp hybrid orbitals of carbon atoms in the respective molecules.

Hybridisation influences the shapes, bond length and bond enthalpy (strength) in compounds. sp^3 -hybridised molecules (alkanes) are tetrahedral in shape, sp^2-hybridised molecules (alkenes) have planar structure and sp -hybridised molecules (alkynes) are linear molecules.

The sp hybrid orbital contains more s character and more the s character more will be the strength of bond. Hence sp hybrid orbital is closer to its nucleus and forms shorter and stronger bonds as compared to sp^3 hybrid orbital. The sp^2 hybrid orbital is intermediate in *s* character between sp and sp^3 and, hence, the length and enthalpy of the bonds it forms are also intermediate between them.

The electronegativity of carbon is also affected by change in hybridisation. More the s character of the hybrid orbitals more will be electronegativity of carbon. Thus, a carbon atom having sp hybrid orbital means 50% s character is more electronegative than that of hybridised carbon. This relative electronegativity is reflected in several physical possessing sp^2 or sp^3 and chemical properties of the molecules concerned. The mixing of atomic orbitals and percentages of s and p character in the corresponding sp^3, sp^2 and sp hybrid orbitals are summarized in table1 shown below.

Table 1

Mixing of atomic orbitals	**Hybrid orbitals and hybridization**	**No. of Hybrid orbitals**	***s*-character**	***p*-character**
one *s* and three *p*	sp^3	4	25%	75%
one *s* and two *p*	sp^2	3	33.3%	66.6%
one *s* and one *p*	sp	2	50%	50%

2.3 Characteristic Features of π (pi) Bonds

In a π (pi) bond formation, parallel orientation of the two p orbitals on adjacent atoms is necessary for a proper sideways overlap. Thus, in $H_2C=CH_2$ molecule all the atoms must be in the same plane. The p orbitals are mutually parallel and both the p orbitals are perpendicular to the plane of the molecule. Rotation of one CH_2 fragment with respect to other interferes with maximum overlap of p orbitals and, therefore, such rotation about carbon-carbon double bond (C=C) is restricted. The electron charge cloud of the p bond is located above and below the plane of bonding atoms. This results in the electrons being easily available to the attacking reagents. In general, p bonds provide the most reactive centres in the molecules containing multiple bonds.

Problem 1

How many s and p bonds are present in each of the following molecules?

(a) $HC{\equiv}CCH{=}CHCH_3$ (b) $CH_2{=}C{=}CHCH_3$

Solution

(a) σ_{C-C}: 4; $\sigma_{C\text{–}H}$: 6; $\pi_{C=C}$:1; $\pi_{C\equiv C}$:2

(b) σ_{C-C}: 3; $\sigma_{C\text{–}H}$: 6; $\pi_{C=C}$:2.

Problem 2

What is the type of hybridisation of each carbon in the following compounds?

(a) CH_3Cl, (b) $(CH_3)_2CO$, (c) CH_3CN, (d) $HCONH_2$, (e) $CH_3CH{=}CHCN$

Solution

(a) sp^3, (b) sp^3, sp^2, (c) sp^3, sp, (d) sp^2, (e) sp^3, sp^2, sp^2, sp

Problem 3

Write the state of hybridisation of carbon in the following compounds and shapes of each of the molecules.

(a) $H_2C{=}O$, (b) CH_3F, (c) $HC{\equiv}N$.

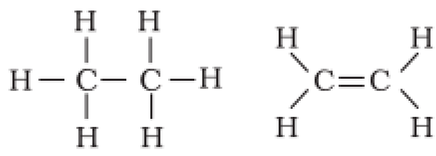
Solution

(a) sp^2 hybridised carbon, trigonal planar; (b) sp^3 hybridised carbon, tetrahedral; (c) sp hybridised carbon, linear.

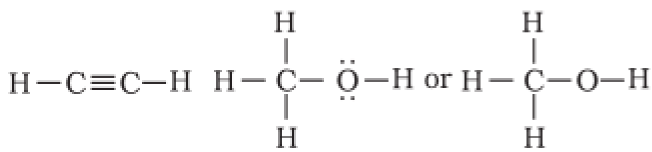
3. Structural Representations of Organic Compounds

3.1 Complete Structural Formulas

There are several ways of representing the structures of organic compounds. Some of the important structural representations are: The Lewis structure or dot structure, dash structure, condensed structure and bond line structural formulas. The Lewis structures can be simplified to dash structure by representing the two-electron covalent bond by a dash (–). Such a structural formula focuses on the electrons involved in bond formation. Single bond is represented by single dash, double bond by double dash and a triple bond by triple dash. Lone pairs of electrons on heteroatoms (e.g., oxygen, nitrogen, sulphur, halogens etc.) may or may not be shown. Thus, ethane (C_2H_6), ethene (C_2H_4), ethyne (C_2H_2) and methanol (CH_3OH) can be represented by the following structural formulas. Such structural representations are called complete structural formulas.



Ethane *Ethene*



Ethyne *Methanol*

3.2 Condensed Structural Formulas

The condensed structural formulas are simplified complete structural formulas. These formulas can be condensed by omitting some or all of the dashes representing covalent bonds and by indicating the number of identical groups attached to an atom by a subscript. The resulting expression of the compound is called a condensed structural formula. Thus, ethane, ethene, ethyne and methanol can be written as:

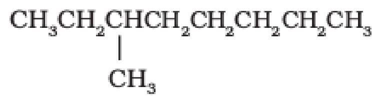
CH_3CH_3	$H_2C{=}CH_2$	$HC{\equiv}CH$	CH_3OH
Ethane	*Ethene*	*Ethyne*	*Methanol*

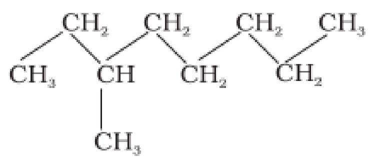
Similarly, $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ can be condensed to $CH_3(CH_2)_6CH_3$ and $CH_3CH_2CH_2CH_2OCH_2CH_2CH_2CH_3$ can be condensed to $CH_3(CH_2)_3O(CH_2)_3CH_3$, which can be further condensed to $(CH_3(CH_2)_3)_2O$.

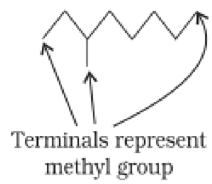
3.3 Bond-line Structural Formulas

Another way of representing the structures of organic molecules is bond-line structural representation. It is most simplified representation of organic molecules. In bond-line structural representation of organic compounds, only lines are used, most importantly, carbon and hydrogen atoms are not shown and the lines representing carbon-carbon bonds are drawn in a zig-zag fashion. The heteroatoms such as oxygen, chlorine, nitrogen etc. are only specifically written. The terminals denote methyl ($–CH_3$) groups (unless indicated otherwise by a functional group), while the line junctions denote carbon atoms bonded to appropriate number of hydrogens required to satisfy the valency of the carbon atoms. Some of the examples are represented as follows:

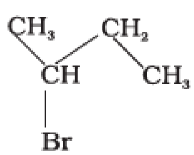
(i) 3-Methyloctane can be represented in various forms as

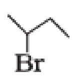
(a) 

(b) 

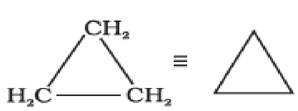
(c) 

(ii) Various ways of representing 2-bromobutane are:

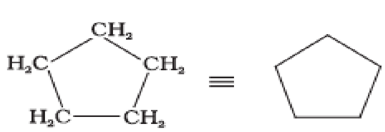
(a) $CH_3CHBrCH_2CH_3$ (b) 

(c) 

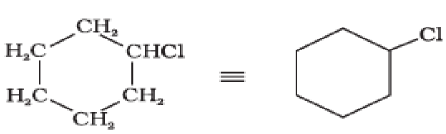
In cyclic compounds, the bond-line formulas may be given as follows:



Cyclopropane



Cyclopentane



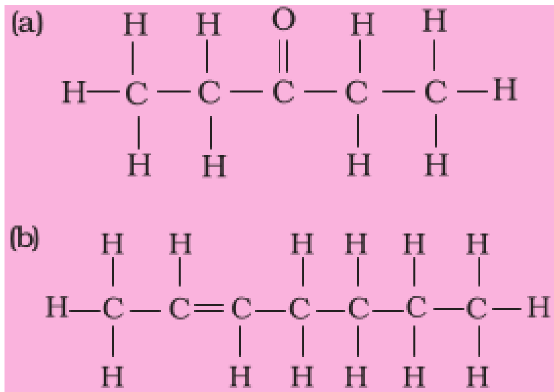
chlorocyclohexane

Problem 4 Expand each of the following condensed formulas into their complete structural formulas.

(a) $CH_3CH_2COCH_3CH_2$

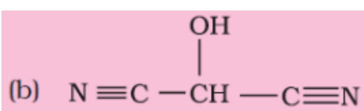
(b) $CH_3CH{=}CH(CH_2)_3CH_3$

Solution



Problem 5 For each of the following compounds, write a condensed formula and also their bond-line formula.

(a) $HOCH_2CH_2CH_2CH(CH_3)CH(CH_3)CH_3$



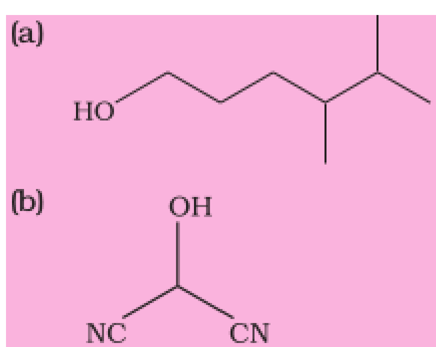
Solution

Condensed formula:

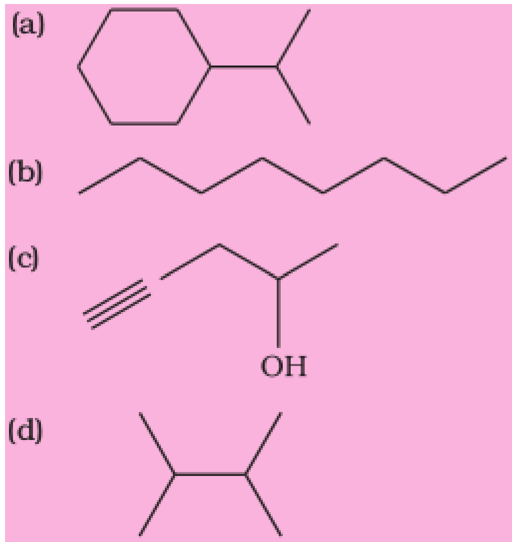
(a) $HO(CH_2)_3CH(CH_3)CH(CH_3)_2$

(b) $HOCH(CN)_2$

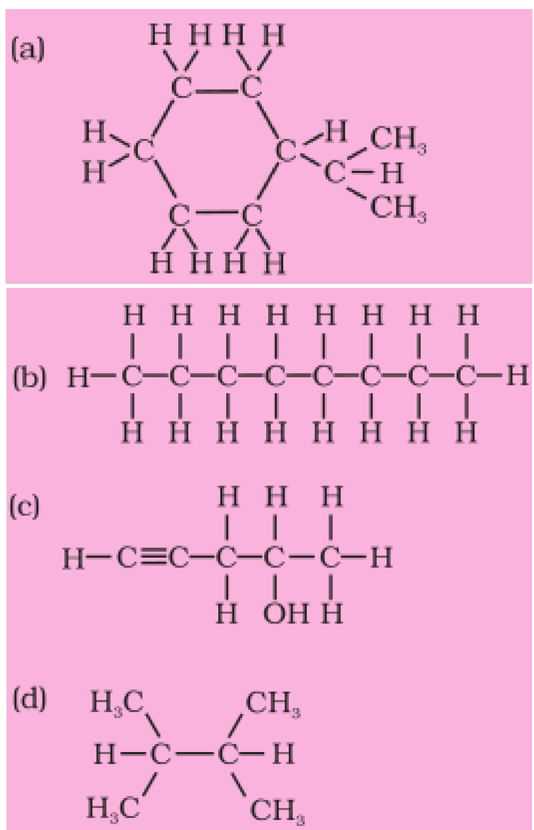
Bond-line formula:



Problem 6 Expand each of the following bond-line formulas to show all the atoms including carbon and hydrogen

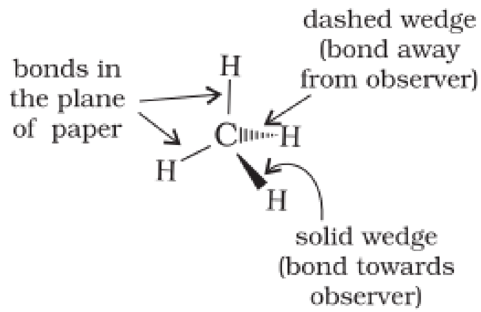


Solution:



3.4 Three-Dimensional Representation of Organic Molecules

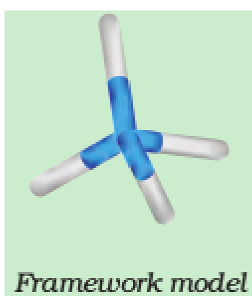
There are some representations which can be used to write three-dimensional (3-D) structure of organic molecules on paper. For example, in wedge formula solid bond (▬) and dashed bond (┆┆┆┆) is used so that the 3-D image of a molecule from a two-dimensional picture can be perceived. In these formulas, a bond out of the plane of paper and towards the observer is indicated by the solid-wedge. However, a bond out of the plane of paper and away from the observer is indicated by the dashed-wedge. Wedges are shown in such a way that the broad end of the wedge is towards the observer. The bonds lying in plane of the paper are depicted by using a normal line (—). 3-D representation of methane molecule on paper has been shown here:



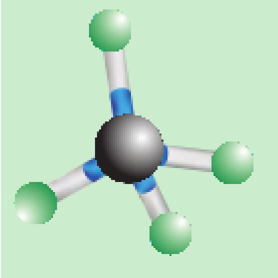
3.5 Molecular Models

Some physical devices can be used for a better visualisation and perception of three-dimensional shapes of organic molecules. These physical devices are called Molecular models. They are made of wood, plastic or metal and are commercially available. Commonly there are three types of molecular models: (1) Framework model, (2) Ball-and-stick model, and (3) Space filling model.

In the framework model, only the bonds are used for connecting the atoms of a molecule but the connecting atoms are not shown. This model only emphasizes on the pattern of bonds of a molecule not on the size of atoms.

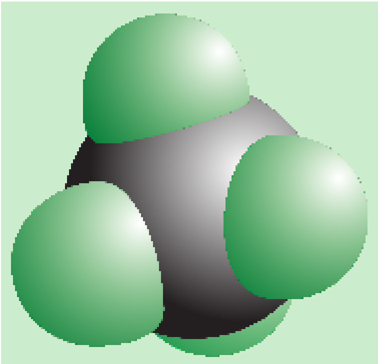


In the ball-and-stick model, the atoms and the bonds both are shown. Balls represent atoms whereas, the stick denotes a bond. Double bond C=C containing compounds (e.g., ethene) can be best represented by using springs in place of sticks. These models are referred to as **ball and spring model**.



Ball and stick model

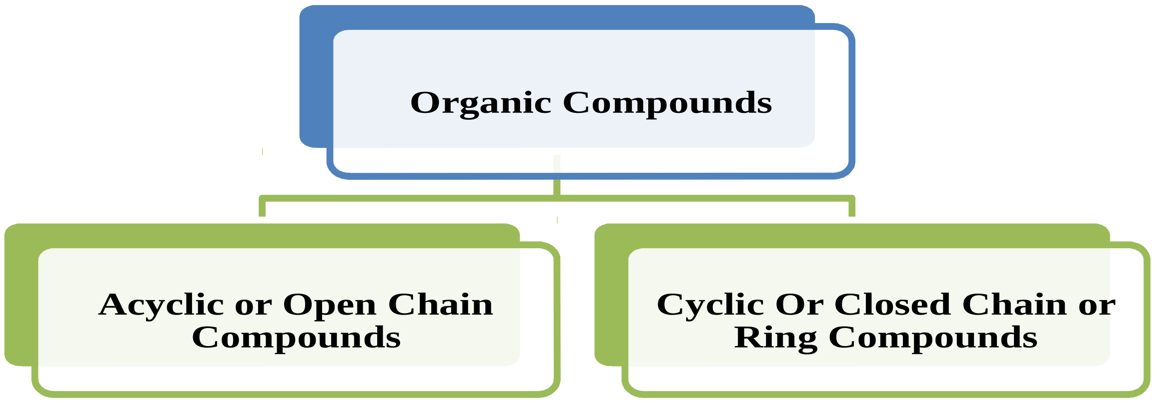
The space-filling model emphasizes the relative size of each atom based on its van der Waals radius. In this model, bonds are not shown and spheres are used to represent the atoms. The radii of spheres are proportional to the radii of the atoms. Spheres of different colors are used for atoms of different chemical elements. This model expresses the volume occupied by each atom in the molecule. In addition to these models, computer graphics can also be used for molecular modelling.



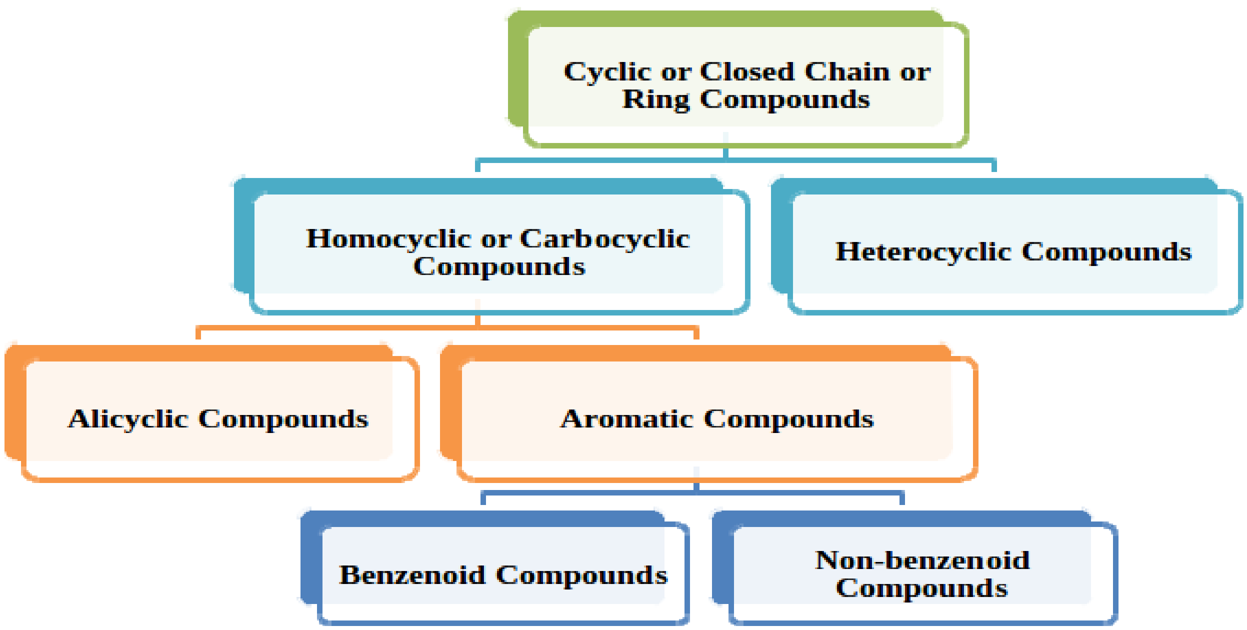
Space filling model

4. Classification of Organic Compounds

The existing large number of organic compounds and their ever-increasing numbers have made it necessary to classify them on the basis of their structures. Organic compounds are broadly classified into: (1) acyclic or open chain compounds and (2) cyclic or closed chain or ring compounds as shown in the flow chart below:



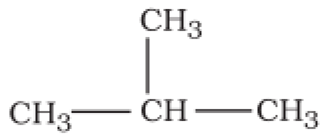
Cyclic or closed chain or ring compounds can be further classified into (i) alicyclic compounds and (ii) aromatic compounds. These are further classified as shown in chart below:

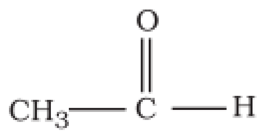


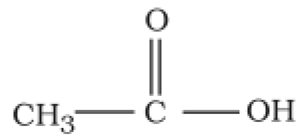
4.1 Acyclic or open chain compounds

The organic compounds consist of straight or branched chains are called acyclic or open chain compounds. Commonly they are also called aliphatic compounds. for example: Ethane, isobutene, acetaldehyde, etc.

CH_3CH_3
Ethane


Isobutane

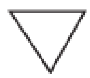

Acetaldehyde

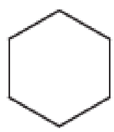

Acetic acid

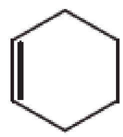
4.2 Cyclic or closed chain or ring compounds

4.2.1 Alicyclic compounds

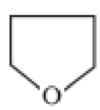
The organic compounds containing carbon atoms joined in the form of a ring are known as alicyclic or aliphatic cyclic compounds. They are also known as homocyclic.


Cyclopropane


Cyclohexane


Cyclohexene

Sometimes atoms other than carbon are also present in the ring (heterocylic). Piperidine and tetrahydrofuran given below are the examples of this type of compound:

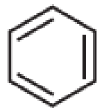
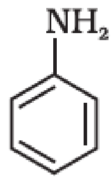
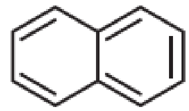

Tetrahydrofuran

These exhibit some of the properties similar to those of aliphatic compounds.

4.2.2 Aromatic compounds

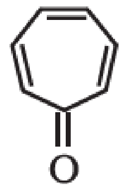
Special organic compounds that contain conjugated planar ring systems with delocalized pi electron clouds. They are also known as arenes or aromatics. These compounds have unique stability. These include benzene and other related ring compounds (benzenoid). Like alicyclic compounds, aromatic compounds may also have hetero atom in the ring. Such compounds are called hetrocyclic aromatic compounds. Some of the examples of various types of aromatic compounds are:

Benzenoid aromatic compounds

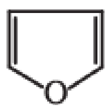
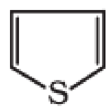
Benzene Aniline Naphthalene

Non-benzenoid compound



Tropone

Heterocyclic aromatic compounds


Furan Thiophene Pyridine

5. Functional Group and Homologous Series

Organic compounds can also be classified on the basis of functional groups, into families or homologous series.

5.1 Functional Group

The functional group is an atom or a group of atoms joined to the carbon chain which is responsible for the characteristic chemical properties of the organic compounds. The examples are hydroxyl group (–OH), aldehyde group (–CHO) and carboxylic acid group (–COOH) etc.

5.2 Homologous Series

A group or a series of organic compounds each containing a characteristic functional group forms a homologous series and the members of the series are called homologues. The members of a homologous series can be represented by general molecular formula and the successive members differ from each other in molecular formula by a $–CH_2$ unit. There are a number of homologous series of organic compounds. Some of these are alkanes, alkenes, alkynes, haloalkanes, alkanols, alkanals, alkanones, alkanoic acids, amines etc. For example, CH_3, C_2H_4, C_3H_6 and soon forms a homologous series. Similarly, CH_3Br, C_2H_5Br, C_3H_7Br and soon forms another homologous series.

It is also possible that a compound contains two or more identical or different functional groups. This gives rise to polyfunctional compounds.

Problem 6 Arrange the following in increasing order of C-C bond length : C_2H_6, C_2H_4, C_2H_2

Solution: $C_2H_2 < C_2H_4 < C_2H_6$

Problem 7 Select the homologous from the following:

CH_3OH, C_2H_4, CH_3Cl, C_3H_6, C_2H_5Cl, C_2H_5OH

Solution: CH_3OH and C_2H_5OH, C_2H_4 and C_3H_6, CH_3Cl and C_2H_5Cl

Problem 8 Select the primary functional group among the following:

(a) –COOH, -OH, -CHO (b) –OH, NO_2, C=C (C) Cl, NO_2, C≡C

Solution: (a) –COOH (b) –OH (C) C≡C

6. **Summary**

- Organic compound is compound whose molecules contain carbon and hydrogen. They are also known as “hydrocarbons”. The derivatives of hydrocarbons are also known as organic compound.
- Hybridisation influences the shapes, bond length and bond enthalpy (strength) in compounds.
- Organic compounds can be represented by various structural representations: Complete Structural Formulas, condensed Structural Formulas and Bond-line Structural Formulas
- Organic compounds can also be represented by 3D-Representation and molecular models
- The three dimensional representation of organic compounds on paper can be drawn by wedge and dash formula.
- Organic compounds can be broadly classified into (1) Acyclic or open chain compounds and (2) Cyclic or closed chain or ring compounds

- Organic compounds can be further classified on the basis of their structure or the functional groups they contain.
- In organic compound, an atom or group of atoms bonded together in a unique fashion is known as functional group that predicts the physical and chemical properties of the compounds.