12. Basic Concepts of Organic Chemistry

Learning outcomes

By the end of this chapter, Students should be able to:

12.1 Define organic chemistry and organic compounds.
12.2 State and explain the origin of organic compounds.
12.3 Describe reasons for the separate study of organic compounds.
12.4 Explain the tetra-covalency and catenation property of carbon.
12.5 Describe the classification of organic compounds.
12.6 Define functional groups and homologous series with examples.
12.7 State and explain the structural formula, contracted formula, and bond line structural formula.
12.8 Introduce preliminary idea of cracking and reforming, quality of gasoline, octane number, cetane number, and gasoline additives.

12.1 Introduction to organic chemistry and organic compounds

- In the early development of chemistry, scientists mainly studied substances obtained from **minerals**. Later, attention shifted to substances like **sugars, fats, oils, and proteins**, which were derived from **plants and animals**.
- The substances of mineral origin were named inorganic, and those of plant and animal origin were called organic.
- Modern research revealed that all organic compounds contain covalently bonded carbon as their essential constituent and are invariably associated with hydrogen.

Hydrocarbons and their derivatives are called organic compounds in which the carbon is covalently bonded.

The branch of chemistry that deals with the study of organic compounds is called organic chemistry.

12.2 Reasons for the separate study of organic compounds from inorganic compounds

(Differences between organic and inorganic compounds.)

Topic	Organic compounds	Inorganic
Source	Mainly living things	Mostly nonliving things
Nature of bond	Mostly covalent	Mostly ionic
Nature of reactions	Slow, **complex**, occur under specific conditions, molecular in nature.	Rapid, **simple**, occur in ordinary conditions, ionic in nature, generally
Elements	C is an essential element, and a few, mainly C, H, O, N, P, S, Cl, Br, I, etc., are present.	Almost all elements
Solubility	Mostly soluble in nonpolar organic solvents and insoluble in polar solvents like water	Mostly insoluble in non-polar organic solvents & soluble in polar solvents like water
Number	There are large numbers of organic compounds, more than 6 million, and new compounds are being discovered each year.	Fewer in number, relatively, nearly a million.
Combustibility	Generally combustible (burn easily)	Generally non-combustible
Melting and boiling points	Generally low	Relatively high

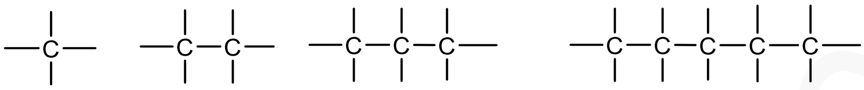
Isomerism	Shown by organic compounds	Generally, not shown

12.3 Tetra-covalency and **Catenation** property of carbon

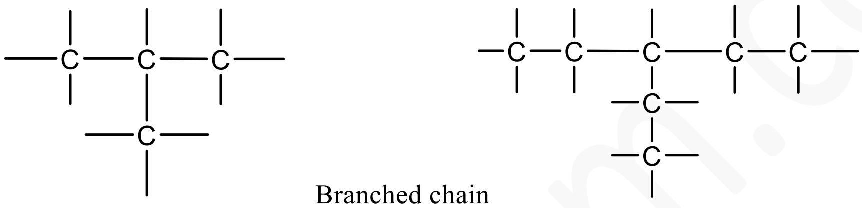
Living things are made up of atoms covalently bonded to form molecules of organic compounds. All these molecules are carbon-based compounds. The complexity of life requires a great variety of compounds. The great variety of compounds is possible because every carbon atom can bond with other atoms to form chains and rings. These chains and rings are often found bonded to atoms of other elements, such as hydrogen, oxygen, and nitrogen. This explains the existence of millions of organic compounds.

- Carbon has 4 electrons in the last shell; it's neither too electropositive nor too electronegative, forming mostly covalent bonds with other nonmetals and itself (i.e., other carbon atoms). Hence, it has **valency four**.

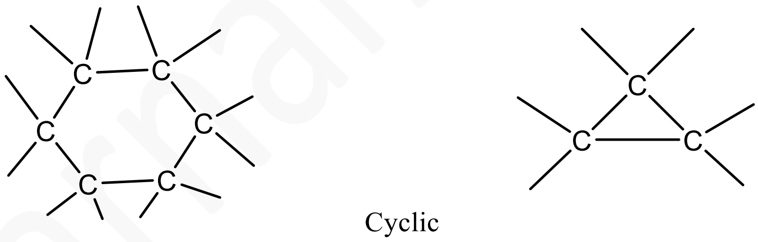
- Another special property of carbon that results in the existence of such a wide variety of organic compounds is the **catenation** property of carbon. It is the property by which carbon gets bonded with another carbon atom, forming a wide variety of possible chains. E.g.,



Straight chains



Branched chain

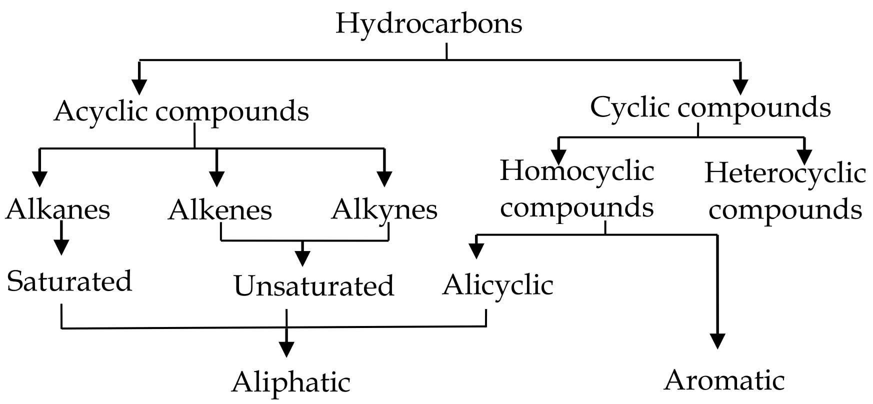


Cyclic

Due to moderate electronegativity and 4 electrons in the valence shell, the carbon-carbon covalent bond is very strong. This is why catenation is very effective in carbon.

12.4 Classification of organic compounds

- The organic compounds made up of hydrogen and carbon atoms only are called hydrocarbons.
- These are considered to be the parent organic compounds, and all other organic compounds are considered to be derived from them by the replacement of one or more hydrogen atoms by other substituents.
- With the development of organic chemistry, the number of organic compounds became very large.
- Therefore, to simplify and systematize the study of organic chemistry, all the known organic compounds are broadly divided into two main classes, viz., hydrocarbons and derivatives of hydrocarbons.
- On the basis of the nature of the carbon skeleton, the hydrocarbons can be classified into cyclic and acyclic.



1. <u>Acyclic or Open Chain Compounds</u>

These are hydrocarbons that contain carbon atoms linked together in an open-chain form. The carbon chain may be a straight chain or branched. E.g.,

$CH_3CH_2CH_2CH_2CH_3$	$CH_3\underset{\displaystyle CH_3}{\underset{\vert}{C}}HCH_2CH_3$
Pentane	2-methylbutane
(Straight chain)	(Branched)

The open-chain compounds can further be classified as alkanes, alkenes, and alkynes.

[A] Alkanes (C_nH_{2n+2})

These are the simplest hydrocarbons, which contain carbon-carbon single bonds. These are also called saturated hydrocarbons as they cannot add any more hydrogen. e.g.

Methane	(CH_4)		16 amu
Ethane	(CH_3CH_3)		30 amu
Propane	($CH_3CH_2CH_3$)		44 amu
Butane	($CH_3CH_2CH_2CH_3$)	C_4H_{10}	58 amu
2-methyl propane	$(CH_3)_2CHCH_3$	C_4H_{10}	etc.
	(12+1 x 3) x 2+12+1+12+1x3 = 58 amu		

[B] Alkenes (C_nH_{2n})

These are unsaturated hydrocarbons that contain at least one carbon-carbon double bond. E.g.,

Ethene	($CH_2=CH_2$)	12x2+1x4=28 amu
Propene	($CH_2=CHCH_3$)	= 42 amu
But-1-ene	($CH_2=CHCH_2CH_3$)	= 56 amu C_4H_8
But-2-ene	($CH_3CH=CHCH_3$)	= 56 amu C_4H_8
Buta-1,3-diene	($CH_2=CHCH=CH_2$) etc.	

[C] Alkynes

These are also unsaturated hydrocarbons that contain at least one carbon-carbon triple bond. E.g.,

$HC\equiv CH$	$HC\equiv C-CH_3$	$HC\equiv C-C\equiv CH$
Ethyne	Propyne	Butadiyne

2. <u>Cyclic or closed chain or ring compounds</u>

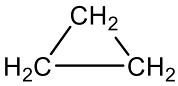
The hydrocarbons that contain one or more rings are called cyclic compounds. These are further divided into the following two categories.

[A] Homocyclic (carbocyclic compounds)

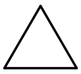
These are closed or ring compounds where the ring is made up of the same atom, i.e., carbon. These are further classified into:

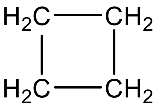
a. Aliphatic Cyclic Hydrocarbons (Alicyclic)

These are closed-chain hydrocarbons but resemble open-chain hydrocarbons in many of their properties. These could be further classified into cycloalkanes, cycloalkenes, and cycloalkynes. e.g.,

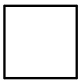


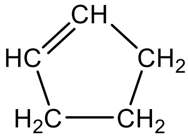
Cyclopropane



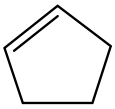


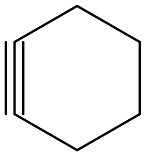
Cyclobutane





Cyclopentene

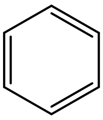




Cyclohexyne

b. Aromatic hydrocarbons

The term aromatic was derived from the Greek word aroma, meaning sweet smell. So, the organic compounds having a sweet smell were originally called aromatic hydrocarbons. Later, it was found that planar cyclic compounds having (4n+2) π electrons in a conjugated system (i.e., alternate single and double bonds) are aromatic compounds. e.g.,



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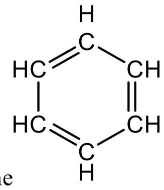
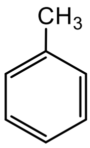
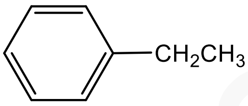


Benzene



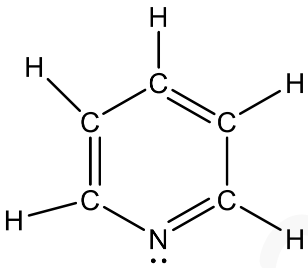
Methyl benzene (Toluene)



Ethyl benzene

[B] Heterocyclic compounds

These are cyclic or ring compounds where, apart from carbon, the ring consists of at least one hetero atom (Oxygen, Sulphur, Nitrogen, etc.). For example,



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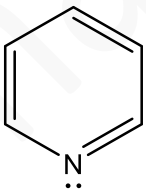
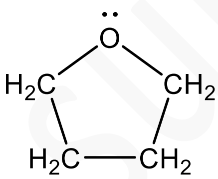


or C_5H_5N

Pyridine



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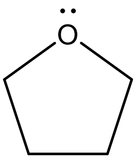


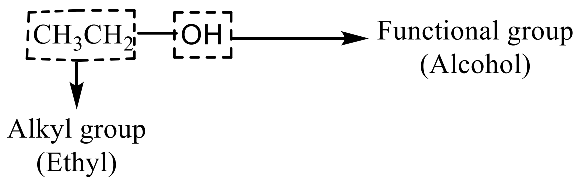
or C_4H_8O

Tetra hydro furan (THF)

etc.

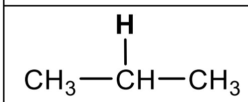
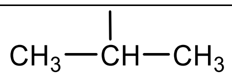
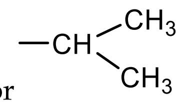
12.5 Alkyl groups, functional groups, and homologous series

Organic compounds except hydrocarbons (i.e., derivatives of hydrocarbons) are generally made up of 2 parts: a skeleton hydrocarbon and another part that determines most of the chemical and physical characteristics of that compound. The latter is called the functional group, and the former one is generally called the alkyl group (-R). e.g.



Alkyl groups (-R)

Alkyl groups can be defined as the **groups obtained by removing one hydrogen atom from an Alkane**.

Parent Alkane	Name	Alkyl group	Name
CH_3-**H**	Methane	$-CH_3$ or CH_3-	Methyl group
CH_3-CH_2-**H**	Ethane	$-CH_2-CH_3$	Ethyl group
$CH_3-CH_2-CH_2$-**H**	Propane	$-CH_2-CH_2-CH_3$	Propyl group (n-propyl group)
	Propane	 or $-CH(CH_3)_2$ or 	1-methylethyl group (iso-propyl group)

Functional groups

The functional group can be defined as the *atom or group of atoms that is present in an organic compound and largely determines the properties* of the compound.

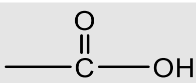
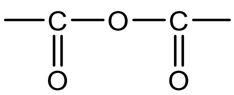
E.g., the properties of Ethanol are entirely different than that of aminoethane, though both have the same alkyl group (ethyl).

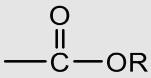
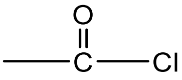
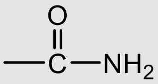
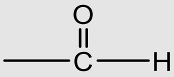
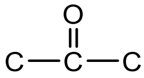
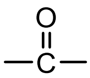
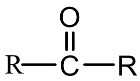
CH_3-CH_2-OH	$CH_3CH_2NH_2$
Ethanol	Aminoethane

On the other hand, most of the properties of Methanol and Ethanol or Aminoethane and Aminomethane are the same.

CH_3-OH	CH_3CH_2OH
Methanol	Ethanol
NH_2CH_3	$NH_2-CH_2-CH_3$
Aminomethane	Aminoethane

There are many functional groups present among organic compounds. A few important ones are listed below.

SN	Functional Group	Name
1	$-SO_3H$	Sulphonic acid
2	-COOH or 	Carboxylic acid
3	-CO-O-CO- or -COOCO- 	Acid anhydride

4	-COOR or  where R is an alkyl group like -CH_3(methyl), -CH_2CH_3(ethyl) etc.	Ester
5	-COCl or 	Acid chloride
6	-$CONH_2$ or 	Amide or acid amide
7	$^{-}$-CN or –C=N	Nitrile or Cyanide
8	-CHO or 	Aldehydes
9	>CO or -CO- or   or 	Ketones
10	–OH	Alcohol
11	-NH_2	Amine or amino
12	-NO_2	Nitro
13	-X (Cl, Br, F etc.)	Halides or halo
14	-O- or R-O-R *or (C-O-C)*	Ether

Homologous series

It is a family or class of compounds obtained when compounds having the same functional group are arranged in increasing order of their molecular weight. It is defined as a **series of organic compounds having the same functional group differing by a –CH_2- unit** or 14 amu weight among successive members. The members of the homologous series are called *homologs,* and the phenomenon is called *homology*.

The main **characteristics** of the homologous series are:

- The members of a homologous series have the **same functional group,** if any.
- They can be represented by a **general formula**.
- They can be prepared by the **same general methods of preparation**.
- They have **similar chemical properties**.
- Each **successive member differs by 14 amu** mass or -CH_2 unit.
- There is **regular gradation in** the **physical properties**.
- The **first member** of the homologous series is generally **different and special**.

12.6 Idea of structural formula, contracted formula, and bond line structural formula

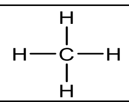
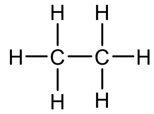
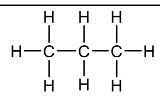
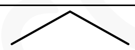
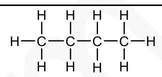
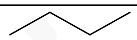
Different representations can be used to indicate organic compounds. The most widely used among them are the structural formula, condensed/contracted formula, and bond line structural formula.

The structural formula shows each atom in the molecule and the nature of the bonds between the different atoms, so it is the clearest one.

The condensed formula is somewhat shorter and uses carbon atoms and hydrogen atoms attached to it as a unit.

The bond line structural formula is the least work to represent an organic molecule; here, a line indicates a single bond between carbon atoms, generally, and the end of the line or corners in the geometrical shape indicate a carbon atom along with hydrogen atoms directly attached to it. Atoms other than these should be written as their symbols.

An example of different representations of molecules of the alkane homologous series, along with names, is presented in the following table.

Name	Molecular formula	Empirical formula	Condensed or contracted formula	Structural formula	Bond line structural formula
Methane	CH_4	CH_4	CH_4		
Ethane	C_2H_6	CH_3	CH_3CH_3		
Propane	C_3H_8	C_3H_8	CH_3-CH_2-CH_3		
Butane (n-butane)	C_4H_{10}	C_2H_5	$CH_3CH_2CH_2CH_3$		

12.7 Preliminary idea of cracking and reforming, quality of gasoline, Octane number, Cetane number, and gasoline additives

1. Pyrolysis or cracking

Coal, petroleum, and natural gases are common sources of hydrocarbons. Generally, *long-chain hydrocarbons* are abundantly found in these sources. But short-chain alkanes and alkenes find more commercial value. Therefore, the long-chain hydrocarbons should be changed into short ones, which is effectively done by pyrolysis or cracking.

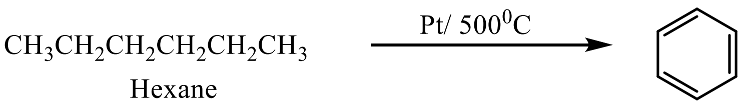
(Greek pyro= fire; lysis= break) Pyrolysis is the **decomposition or breaking of a substance (long-chain hydrocarbons) by using heat.**
Long chain alkanes, when heated in the absence of air to a temperature 500-600^{0}C, decompose into lower alkanes and alkenes. A mixture of lower alkanes and alkenes is obtained by this process.

$C_{10}H_{22}$ (Decane) →

- $C_5H_{12} + C_5H_{10}$ (Pentane, Pent-1-ene)
- $C_6H_{14} + C_4H_8$ (Hexane, But-1-ene)
- $C_7H_{16} + C_3H_6$ (Heptane, Propene)
- $C_8H_{18} + C_2H_2$ (Octane, Ethene)
- $C_7H_{14} + C_3H_8$ (Hept-1-ene, Propane)
- $C_6H_{12} + C_4H_{10}$ (Hex-1-ene, Butane) etc.

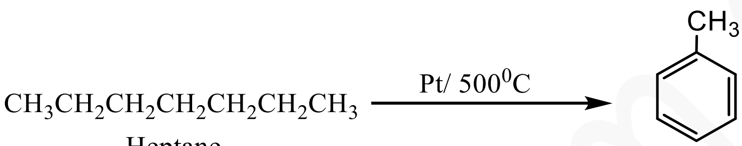
Reforming (Aromatisation)

When **alkanes having 6-8 carbon atoms are heated at a temperature of about 500^{0}C in the presence of Pt, aromatic hydrocarbons are obtained**. These reactions are aromatisation or reforming. This is **done to increase the octane number** of gasoline as well as **fulfil the demand for aromatic compounds**.



Hexane
(n-hexane)

Benzene



Heptane
(n-heptane)

Methyl benzene
(Toluene)

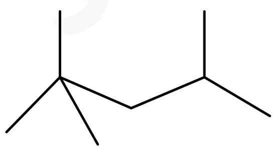
Quality of Gasoline

In a petrol engine, a mixture of petrol and air is compressed in the cylinder. The fuel burns just before the completion of the compression. But if the quality of fuel is not good, combustion takes place before the spark plug ignites, and the piston is pushed suddenly, producing a metallic noise which is called knocking. Knocking reduces efficiency and the life span of the engine.

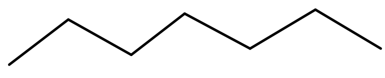
Octane Number

It is a number assigned to grade the quality of gasoline (petrol). Octane number of a fuel (gasoline) is defined as the **percentage of iso-octane in a mixture of *iso-octane* and *n-heptane* which has the same knocking property as the given fuel**. E.g., a fuel has an octane number of 70 means that it has the same anti-knocking properties as a mixture of 70% iso-octane and 30% n-heptane.

The bond line structures of iso-octane and n-heptane are:



2,2,4-trimethylpentane (iso-octane)



Heptane (n-heptane)

Generally, straight-chain hydrocarbons have a lower octane number, and branched-chain hydrocarbons have a higher octane number.

Cetane Number

Similar to the octane number of gasoline, the cetane number of diesel is defined as the **% of n-cetane in the mixture of n-cetane and *a-methylnaphthalene*, having the same *time lag* for ignition as the fuel (diesel) under consideration**.

n-cetane is Hexadecane ($C_{16}H_{34}$) a straight chain saturated hydrocarbon(alkane).

Gasoline additives (Anti-knocking Agents)

- The compounds added to gasoline to reduce the fuel's knocking tendency are called gasoline additives or anti-knock agents.
- Tetraethyl lead (TEL) was one of the most common anti-knock agents.
- But due to its pollution and adverse effects on human health, the use of TEL has been phased out worldwide (2021).

Modern alternatives (oxygenates and other hydrocarbons):

- **MTBE** (methyl *tert*-butyl ether) – good octane booster but causes groundwater pollution (banned in many countries).
- **Ethanol** – widely used, renewable, high octane, but lowers fuel energy density.
- **Aromatics** (toluene, xylene) – boost octane but increase soot and benzene emissions.

Chapter Summary

- Study of **carbon-containing compounds** (mainly with H, O, N, etc.)
- **Organic compounds** = hydrocarbons and their derivatives. Characterised by **covalent bonding**

◆ **Organic vs Inorganic (Key Differences)**

- **Organic:** Covalent, complex, slow reactions, low m.p./b.p, combustible
- **Inorganic:** Ionic, simple, fast reactions, high m.p./b.p, non-combustible

◆ **Properties of Carbon**

1. Tetravalency: Carbon forms **4 covalent bonds**

2. Catenation: Ability to form **chains, branches, and rings**

- Due to **strong C–C bonds**

◆ **Classification of Organic Compounds**

1. Hydrocarbons

- **Alkanes (C_nH_{2n+2})** → Single bond (saturated)
- **Alkenes (C_nH_{2n})** → Double bond
- **Alkynes (C_nH_{2n-2})** → Triple bond

2. Structure-Based

- **Acyclic (Open chain)** → Straight/branched
- **Cyclic (Closed chain):**
  - **Homocyclic** → Only carbon
  - **Heterocyclic** → Contains O, N, S
  - **Aromatic** → Follow (4n+2) π rule

◆ **Functional Group & Alkyl Group**

- **Functional group:** Determines properties (–OH, –COOH, $-NH_2$, etc.)
- **Alkyl group (–R):** Derived from alkanes (CH_3-, C_2H_5-)

◆ **Homologous Series**

- Same functional group — Differ by **$-CH_2$ (14 amu)**
- Show **similar chemical properties** — Gradual change in physical properties

◆ **Representation of Compounds**

- **Structural formula** → Full detail
- **Condensed formula** → Short form

- **Bond-line formula** → Simplified (used most)

◆ **Petroleum & Fuel Concepts**

Cracking: Break long hydrocarbons → smaller ones (500–600°C)

Reforming: Convert alkanes → aromatics (increase fuel quality)

◆ **Fuel Quality**

- **Knocking:** Premature combustion in engines

Octane Number (Petrol)

- Measures **anti-knocking property**

Cetane Number (Diesel)

- Measures **ignition quality**

◆ **Additives:** Improve fuel performance

- Example: **Tetraethyl lead (TEL)** (now banned due to toxicity)

*** ... ***