3

Chemical Stoichiometry

3.1 INTRODUCTION

We know that atoms react to form molecules in simple whole-number ratios. For example, hydrogen and oxygen atoms combine in a two is to one (2:1) ratio to from water, H_2O. However, it is impossible to deal with individual atoms because they are tiny. In a real laboratory situation, we must increase the size of these quantities to the point where we can see them and weigh them. With the help of **mole concept** it is possible to take a desired number of atoms/molecules by weighing. (please refer to lesson-2). Now in order to study chemical compounds in the laboratory, it is necessary to have knowledge of the quantitative relationship that exists among the amount of the substances that take part in the chemical reaction. **Stoichiometry** (derived from the Greeks Stoicheion = element and metron = measure) is the term we use to refer all the quantitative aspects of chemical compounds and reactions. In the present lesson, you will see how chemical formulae are determined and how chemical equations prove useful in predicting the proper amounts of the reactants that must be mixed to obtain a complete reaction. In other words, we can take reactants for a reaction in such a way that none of the reacting substances is in excess. This aspect is very vital in chemistry and has wide application in industries.

3.2 OBJECTIVES

After reading this lesson, you will be able to

- Define empirical and molecular formulae.
- Differentiate between empirical and molecular formulae.
- Calculate prcentage by mass of an element in a compound and also work out empirical formula from the percentage composition.
- Provide atomic, molar and mass interpretation of formula a compound (compound stoichiometry)
- Calculate the amount of substances consumed or formed in a chemical reaction (using a balanced equation and mole concept).

* Formulae is plural of formula

- Explain that the amount of a limiting reagent present initially limits the amount of the products formed.

3.3 MOLECULAR AND EMPIRICAL FORMULAE

In your previous classes, you have studied how to write a chemical formula of a substance. For example, water is represented by H_2O, carbon dioxide is represented by CO_2, methane is represented by CH_4, nitrogen pentaoxide is represented by N_2O_5, and so on. You are aware, formula for a molecule uses a symbol and subscript number to indicate the number of each kind of atoms in the molecule (subscript 1 is always omitted). Such a formula is called **molecular formula** as it represents a molecule of a substance. A molecule of water consists of two hydrogen atoms and one oxygen atom. So its molecular formula is written as H_2O. Thus a molecula formular shows the actual number of atoms of different elements in a compound.

There is another kind of formula, the **empirical formula,** which gives only relative number of atoms of different elements in a compound. These numbers are expressed as the simplest ratio. For example, empirical formula of glucose, which consists of carbon, hydrogen and oxygen in ratio of 1:2:1 is CH_2O (empirical formulae are also called simplest formulae). Molecular formula of a substance is always an integral multiple of its empirical formula (i.e. molecular formula = nx where x is empirical formula and n is an integer). For example molecular formula of glucose is $C_6H_{12}O_6$ which is 6 × its empirical formula. Thus, while empirical formula gives only a ratio of atoms, the molecular formula gives the actual number of atoms of each element in an individual molecule. In some cases the ratio of atoms shown in a molecular formula cannot be reduced to smaller integers. In such cases molecular and empirical formulae are the same, for example, sucrose $C_{12}H_{22}O_{11}$ which is popularly known as canesugar. In case of certain elements, a molecule consists of several atoms for example P_4, S_8, etc. In such cases, empirical formula will be symbol of the element only.

As you know, common salt, which is chemically called sodium chloride is represented as NaCl. This salt is ionic in nature and does not exist in molecular form. Therefore, NaCl is its empirical formula which shows that Sodium and Chlorine and NaCl are present in the ratio of 1:1. Similar is the case with other ionic subtances.

KCl, $NaNO_3$, MgO are examples of empirical formulae as these are ionic compounds. Table 3.1 provides a few more examples.

Table 3.1 Molecular and empirical formulae

Substance	Molecular formulae	Epirical formulae
Ammonia	NH_3	NH_3
Carbon dioxide	CO_2	CO_2
Ethane	C_2H_6	CH_3
Fructose	$C_6H_{12}O_6$	CH_2O
Sulphur	S_8	S
Benzene	C_6H_6	CH
Sodium chloride	—	NaCl
Calcium oxide	—	CaO

3.4 CHEMICAL COMPOSITION AND FORMULAE

How much carbon is present in one kilogram of methane whose molecular formula is CH_4?

How much nitrogen is present in one kilogram of ammonia, NH_3? If we have prepared a substance that is made of 58.8% carbon, 28.4% oxygen, 8.28% nitrogen and 6.56% hydrogen, what is its empirical formula? You have studied **atomic masses, formulae,** and the **mole concept.** Can you solve the problem using these basic concepts? The answer is 'yes'. Atomic masses, formulae and the mole concept are the basic tools needed to solve such problems. What is percentage composition? Let us take up this aspect in a little detail and try to understand.

3.4.1 Percentage composition

If we know the formula of a compound, we can find out how much of each of the elements is present in a given amount of the compound. Aluminium is obtained from its oxide, Al_2O_3 (which is found as the ore, bauxite).

From the formula we can calculate how much aluminium can be obtained, at least in principle, from a given amount of aluminium oxide. Calculation is done by making use of the idea of **percentage composition** which is the percentage of the total mass of a compound contributed by each element.

percentage mass of an element in a compound

$$\frac{\text{mass of element in one molecular formula or one empirical formula}}{\text{molecular mass or empirical formula mass of compound}} \times 100$$

$$= \frac{\text{Mass of element in 1 mol compound}}{\text{Molar mass of compound}} \times 100$$

Let us calculate percentage composition of aluminium oxide, Al_2O_3

$$\text{Percent aluminium} = \frac{\text{Mass of aluminium in 1 mol } Al_2O_3}{\text{Molar mass of } Al_2O_3} \times 100\%$$

Molar mass of $Al_2O_3 = (2 \times 27.0) + (3 \times 16.0)\text{g} = 102.0 \text{ g}$

Since 1 mol of Al_2O_3 contains 2 mol of Al atoms, the mass of Al is $2 \times 27.0 \text{ g} = 54.0 \text{ g Al}$

$$\text{Percentage of Aluminium} = \frac{54.0\text{g}}{102.0\text{g}} \times 100\% = 52.9\%$$

We can calculate percentage of oxygen in the same way. One mole of Al_2O_3 contains 3 mole of O atoms, therefore

$$\text{Percentage oxygen} = \frac{3 \times 16.0\text{g}}{102.0\text{g}} \times 100\% = 47.0\%$$

Example 3.1: Butyric acid, has the formula $C_4H_8O_2$. What is the elemental analysis of butyric acid?

Solution: Molecular formula of the butyric acid is $C_4H_8O_2$.

In one mole of butyric acid there are 4 mol of carbon atoms, 8 mol of hydrogen atoms and 2 mol of oxygen atoms. Thus, 1 molar mass of butyric acid will be equal to the sum of 4 × molar mass of carbon atoms, 8 × molar mass of hydrogen atoms, and 2 × molar mass of oxygen atoms or 1 molar mass of butyric acid $= 4 \times 12.0\ 1\text{g} + 8 \times 1.0 \text{ g} + 2 \times 16.0 \text{ g} = 88.0 \text{ g}$

$$\text{Percentage of C by mass} = \frac{48.0 \text{ g}}{88.0\text{g}} \times 100\% = 54.5\%$$

$$\text{Percentage of H by mass} = \frac{8.0\text{g}}{88.0\text{g}} \times 100\% = 9.1\%$$

$$\text{Percentage of O by mass} = \frac{32.0\text{g}}{88.0\text{g}} \times 100\% = 36.4\%$$

3.5 DETERMINATION OF EMPIRICAL FORMULAE — FORMULA STOICHIOMETRY

We have just seen that if we know the formula of a compound we can calculate the percentage composition. Now the question arises can we determine the formula of the compound if we know the percentage of a composition? The answer will be 'yes', but this formula will not be molecular formula; instead it would be **empirical formula** as it gives relative number of atoms present in a compound. Normally we determine the percentage composition of different elements present in an **unknown compound** and determine its formula. Let us take a simple example of water. Water is 11.19% hydrogen and 88.81% oxygen by mass. From the data, we can determine empirical formula of water Now if we assume that we have a 100.00 g sample of water, then the percentage composition tells us that 100.0 g of water contains 11.19 g of hydrogen atoms and 88.81 g of oxygen atoms.

From the atomic mass table, we find that 1 mol of hydrogen atoms has a mass of 1.0 g, and 1 mol of oxygen atoms has a mass of 16.0 g. Now we can write **unit conversion factors** so that the mass of hydrogen can be converted to moles of H atoms and the mass of oxygen can be converted to moles of O atoms. Since 1 mol of H atoms has a mass of 1.0 g we get the conversion factor as

$$\frac{1\,\text{mol H atoms}}{1.0\,\text{g H}}$$

Therefore

$$11.19\text{ g H} = (11.19\text{ g H})\frac{1\,\text{mol H atoms}}{1.0\,\text{g H}} = 11.1\,\text{mol H atoms}$$

Similarly conversion factor for oxygen will be

$$\frac{1\,\text{mol O atoms}}{16.0\,\text{g O}}$$

$$\text{Therefore, } 88.81\text{ g O} = (88.81\text{g O})\frac{1\,\text{mol O atoms}}{16.0\text{ g O}} = 5.55\,\text{mol O atoms}$$

Thus in water, the ratio of moles of hydrogen atoms to moles of oxygen atoms is 11.10:5.55

Since a mole of one element contains the same number of atoms as a mole of another element, the ratio of moles of atoms in a compound is also the ratio of the number of atoms. Therefore the ratio of hydrogen atoms to oxygen atoms is 11.10:5.55. Now by dividing each by the smaller of the two numbers we can convert both numbers to integers.

$$\frac{11.10}{5.55} = 2 \text{ and } \frac{5.55}{5.55} = 1$$

Thus, ratio of H atoms to O atoms is 2:1, and the empirical formula of water is therefore H_2O. If we know molecular mass, we can also calculate the molecular formula of the compound. Experimentally it is found that molecular mass of the water is the same as empirical formula mass. In other words, empirical and molecular formula in case of water is the same. However in the case of ethane the empirical formula is CH_3 and formula mass is 15.0 amu whereas Molecular mass of ethane (experimentally determined) is 30.0 amu. Now ratio of the molecular mass to empirical formula mass (i.e. molecular mass/empirical formula mass) is 2. Therefore, molecular formula of ethane is $2 \times (CH_3)$ or C_2H_6. Thus, if the empirical formula is known, then determination of molecular formula will only be possible if molecular mass of the substance is known.

Here it would be quite necessary to remind you that in water, hydrogen and oxygen atoms are present in a definite ratio. Using mole concept we can say that in one mol of H_2O, there are 2 mol atoms of hydrogen and 1 mol atoms of oxygen. In other words in one molar mass i.e. 18.0 g of water (H_2O) there is 16.0 g of oxygen and 2.0 g of hydrogen. This aspect of study falls under **compound stoichiometry.** You can take different compounds and work out their stoichiometry using atomic masses, molecular masses and mole concept.

INTEXT QUESTIONS: 3.1

1. For the compound Fe_3O_4, calculate percentage of Fe and O.

   ....

2. State percent composition for each of the following:

   (a) C in $SrCO_3$ (b) SO_3 in H_2SO_4

   ....

3. What are the empirical formulae of substances having the following molecular formulae?

   H_2O_2, C_6H_{12}, Li_2CO_3, $C_2H_4O_2$, S_8 H_2O, B_2H_6, O_3, S_3O_9, N_2O_3

   ....

4. A compound is composed of atoms of only two elements, carbon and oxygen. If the compound contain 53.1% carbon, what is its empirical formula.

   ....

3.6 CHEMICAL EQUATION AND REACTION STOICHIOMETRY

You have studied that a reaction can be represented in the form of a chemical equation. Qualitatively, a chemical equation simply describes what the reactants and products of a reaction are. For example

$$4Fe(s) + 3O_2(g) \rightarrow 2Fe_2O_3(s) \qquad ...(3.1)$$

describes a reaction in which iron reacts with oxygen to form iron oxide. Quantitatively, a balanced chemical equation specifies numerical relationship among the qualities of reactants and products of a reaction. These relationships can be expressed in terms of microscopic quantities viz., atoms, molecules, formula units, etc., or macroscopic quantities viz moles of atoms, molecules, formula units etc. The equation (3.1) has actually two qualitative meaning:

First that 4 iron atoms combine with 3 oxygen molecules to form 2 iron oxide formula units and second that 4 mol of iron atoms combine with 3 mol of oxygen molecule to form 2 mol of iron oxide units.

The coefficient in the balanced equation describes fixed ratios among the quantities of reactants and products.

let us take chemical equation for combustion of butane

$$2\,C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O \qquad ...(3.2)$$

Here, above equation can be interpreted in the following ways:

i) 2 molecules of C_4H_{10} + 13 molecules of O_2 → 8 molecules of CO_2 + 10 molecules of H_2O

or

ii) 2 mol of C_4H_{10} + 13 mol of O_2 → 8 mol of CO_2 + 10 mol of H_2O

If we compute the molar masses of different substances in the reaction and multiply each by the number of moles representing the balance equation, we can write,

116.0 g of C_4H_{10} + 416.0 g of O_2 → 352.0g of CO_2 + 180.0 g of H_2O

A balanced equation thus gives a quantitative relationship between the masses of reactants and products.

Thus, we have seen that strochiometry is based on chemical equation and on relationship between mass and mole. Such calculations are fundamental to most quantitative work in chemistry.

3.6.1 Molar Interpretation of Chemical Equations (Revisited):

Let us consider manufacture of ammonia by Haber's process. We know that nitrogen reacts with hydrogen at high temperature and pressure in the presence of a catalyst and gives ammonia.

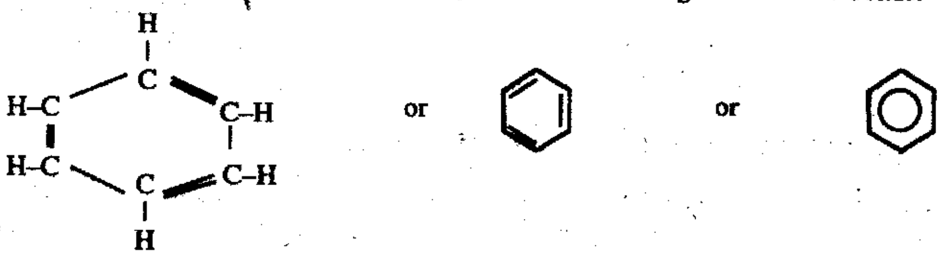
$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g) \qquad ... (3.3)$$

Perhaps you might be aware, hydrogen is obtained from natural gas or petroleum and so it is relatively expensive. For this reason, the price of hydrogen partly determines the price of ammonia. Suppose some one asks you, how much hydrogen would be needed to produce one metric tone of ammonia? Similar questions arise throughout chemical research and industry. For each quantitative questions, we must look again at the chemical equation

$N_2(g)$	+	$3H_2(g)$	→	$2NH_3(g)$	
1molecule of nitrogen	+	3 molecules of hydrogen	→	2 molecules of ammonia	**(Molecular interpretation)**
or $1 \times 6.022 \times 10^{23}$ molecules of N_2	+	$3 \times 6.022 \times 10^{23}$ molecules of H_2	→	$2 \times 6.022 \times 10^{23}$ molecules of NH_3	
or 1 mole of N_2	+	3 mol of H_2	→	2 mol of NH_3	**(Molar interpretation)**
or 28.0 g of nitrogen	+	3×2.0g of hydrogen	→	2×17.0g of ammonia	**(Mass interpretation)**

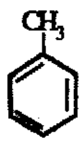
Suppose we ask how many grams of nitrogen will react with 6.0 g of hydrogen, we see

(b) Aromatic hydrocarbons: These hydrocarbons are collectively known as **arenes**. They contain one or more hexagonal carbocyclic rings. The name aromatic is devived from the Greek word 'aroma' meaning sweet smell because most of the compounds belonging to this class have sweet fragrance. One of the earliest aromatic hydrocarbons known is benzene. The benzene ring has six carbon cyclic chain with single and double bonds.



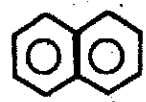
Benzene

Other aramatic Compounds are derived from benzene. Some of the examples are:



Toluene

Xylene



Napthalene

In brief, the classification of hydrocarbons can be given as follows:

- Hydrocarbons
  - Acyclic or Aliphatic Hydrocarbons
    - Alkanes
    - Alkenes
    - Alkynes
  - Carbocyclic or Cyclic Hydrocarbons
    - Alicyclic Hydrocarbons
      - Cyclo Alkanes
      - Cycloalkenes
      - Cycloalkyne
    - Aromatic Hydrocarbons

INTEXT QUESTIONS 25.1

1) Write three categories of Aliphatic Hydrocarbons.

....

2) Give one example of

   i) Alicyclic hydrocarbon

   ii) Aromatic hydrocarbon

....

25.4 IUPAC NOMENCLATURE

The term nomenclature means the system of naming of organic compounds. In the begining of organic chemistry, the organic compounds were named after the source from which they were prepared e.g. methane was named as marsh gas as well as damp fire. These names of organic compound are called common names or trivial names. There was no systematic basis for naming them. In order to bring uniformity and rationality in naming the organic compounds throughout the world, International Union of Chemists came out with a system of nomenclature known as International Union of Pure and Applied Chemistry (IUPAC) system. This system is widely accepted and has rules for naming organic compounds. Let us discuss the nomenclature of hydrocarbons.

25.4.1 Nomenclature of Acyclic Hydrocarbons

a) **Straight chain Hydrocarbons:** To name these types of Hydrocarbons, we generally take care of two aspects. The first one is word root and second one is suffix. Word root designate the number of carbon atoms in the chain. Special word roots are used for chains containing one to four carbon atoms but for chains of five and more carbon atoms, Greek number roots are used. IUPAC word root for a few carbon chains are as follows.

Chain Length	Word root	Chain Length	Word root
C 1	Meth –	C 6	Hex –
C 2	Eth –	C 7	hept –
C 3	Prop –	C 8	Oct –
C 4	But –	C 9	Non –
C 5	Pent –	C10	Dec –

The general word root for any carbon chain is alk.

In order to write IUPAC name, a suffix is added to the word root to indicate saturation or unsaturation in the hydrocarbons. These suffixes are as under.

Class of compound	Suffix	General name
Saturated	– ane	Alkane
Unsaturated (>C = C<)	– ene	Alakene
Unsaturated (–C ≡C–)	– yne	Alkyne

Let us take some examples:

CH_4 – Methane i.e., Meth word root, ane suffix

$CH_3 - CH_2 - CH_3$ Propane i.e., prop word root, ane suffix

$CH_2 = CH_2$ Ethene i.e., Eth. word root, ene suffix

$CH_3 - C \equiv CH$ Propyne i.e., Prop word root, yne suffix

b) Nomenclature of branched chain Hydrocarbons

In branched chain hydrocarbons, the carbon atoms are present in the side chain along with the straight chain of carbon atoms. The carbon atoms inside the chain constitute **alkyl groups or alkyl radicals** These alkyl groups are expressed as prefixes in the IUPAC name. An alkyl group is obtained from an alkane by removing one hydrogen atom. Since the general formula of alkane is C_nH_{2n+2}, the general formula of alkyl group is C_nH_{2n+1}. The alkyl group is generally represented by R-. The alkyl radicals is named by replacing suffix **ane** from the name of the corresponding alkane by yl. Let us see some of the examples of alkl group in the following tables.

Parent Chain	Formula R – H	Alkyl group R –	Name
Methane	CH_4	CH_3-	Methyl
Ethane	CH_3CH_3	$CH_3\,CH_2-$	Ethyl
Propane	$CH_3CH_2CH_3$	$CH_3CH_2CH_2-$	1- Propyl (n-Propyl
		$CH_3-CH-CH_3$	2-Propyl (Iso-Propyl
Butane	$CH_3CH_2CH_2CH_3$	$CH_3CH_2CH_2CH_2-$	1-Butyl (n-Butyl)
		CH_3CH-CH_2 with CH_3 on CH	2-Butyl or Sec Butyl or Iso Butyl
Isobutane	$CH_3-CH(CH_3)-CH_2$	$CH_3-C(CH_3)(CH_3)-$	Tert. Butyl

Branched chain hdrocarbons are named using the following rules in IUPAC system.

Rule 1- Longest chain Rule: According to this rule, the longest possible chain of carbon atoms is picked up and the compound is named as derivative of this alkane. If some multiple bond is present, the selected chain must contain the carbon atoms of the multiple bond. The number of carbon atoms in the selected chain determines the word root and the saturation or unsaturation will determine the primary suffix.

For Example :

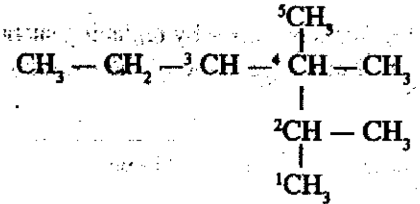
$$CH_3-CH_2-CH_2-\underset{\displaystyle CH_2-CH_3}{\underset{|}{CH_2}}-CH_2-CH_3$$

Wordroot — Hex Suffix —ane

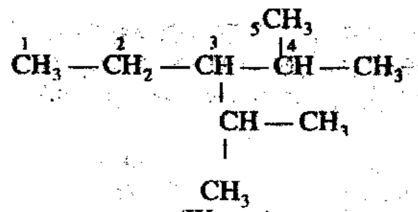
$$CH_3-CH-\overset{\displaystyle CH_3}{\overset{|}{}}\!\!\underset{\displaystyle CH_2}{\underset{\|}{C}}-CH_2-CH_3$$

Wordroot — but
Suffix — ene

If two equally long chains are possible, the chain with maximum number of side chains is selected.



Word root - Pent
Suffix - ane
(Correct)



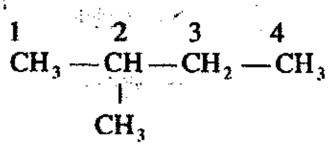
(Wrong)

Rule 2: Lowest number or lowest sum rule : The carbon chain is numbered from one end to another by arabic numerals and the positions of the side chain are indicated by the number of C-atoms to which these are attached. The numbering is done in such a way that :

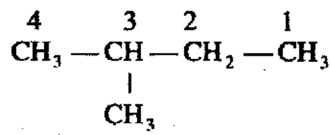
a) The substituted carbon atoms have the lowest possible numbers.

b) The sum of numbers used to indicate the positions of various alkyl groups must be the lowest.

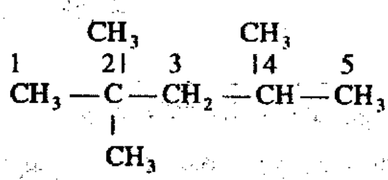
c) If some multiple bond is present in the chain the carbon atoms involved in the multiple bond should get the lowest possible numbers. For Example :



Correct

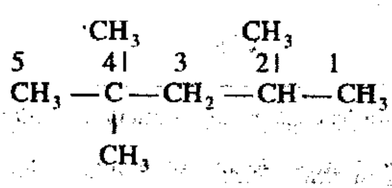


Wrong



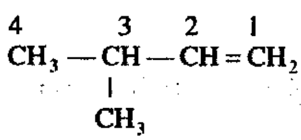
Sum of positions = 2 + 2 +4 = 8

Correct

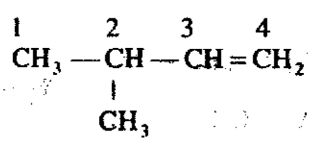


Sum of positions = 2 + 4 + 4 = 10

Wrong



Correct

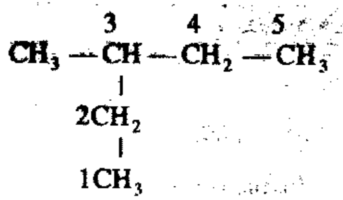


Wrong

The name of the compound in general is written in the following sequence.

Position of substituent — Name of substituent, Word root, Suffix.

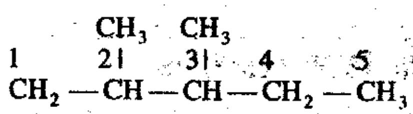
For example the name of the compound



is written as 3-methyl pentane. The substituent is ***Methyl*** group at position number 3. The word root is **Pent** and suffix **is ane.**

Rule 3: Naming the same Alkyl groups at different positions.

If the compound contains more than one similar alkyl groups, their positions are indicated separately and prefix di (two) tri (three) is attached to the name of the substituents. The position of the substituents is seperated by commas (,).

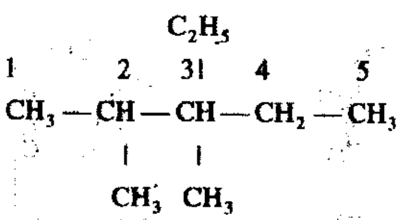


2,3 Dimethyl pentane.

Rule 4: Naming different Alkyl substituent.

If there are different alkyl substituents present in the compound, their names are written in the alphabatical order, However, prefixes di, tri, etc are not considered in order of preferance.

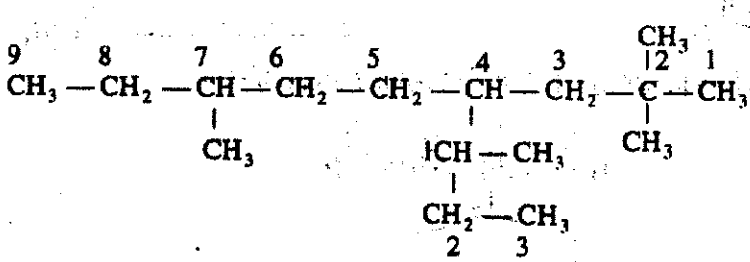
For Example



3 – Ethyl — 2, 3 — dimethyl pentane

Rule 5: Naming of complex alkyl substituent.

If alkyl substituent is further branched, it is named as substituted alkyl group. For this purpose, the carbon atoms of the alkyl groups are seperately numbered in such a way, that the carbon atom directly attached to the parent chain is given the number. The name of such substituent is enclosed in brackets as shown below.



2,2,7-Trimethyl-4(1– methyl propyl) nonane

IN TEXT QUESTIONS-25.2

1. Write word root and suffix of
   i) Six carbons and all single bonds
   ii) Five carbons and one double bond
   iii) Three carbons and one triple bond

   ....

2. Name two rules used for naming hydrocarbons in IUPAC System.

   ....

3. Write the sequence used for naming the branched chain hydrocarbon.

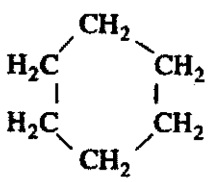
   ....

25.4.2 Nomenclature of Cyclic Hydrocarbons

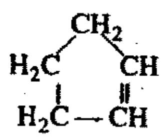
As we already know that cyclic hydrocarbons are divided under two categories of compounds i.e. alicyclic and aromatic compounds. Now let us learn to name these compounds one by one.

a) Naming the alicyclic compunds.

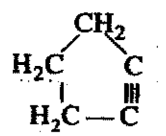
These compounds are cyclic i.e. have closed chain, hence names of alicyclic compounds are derived by putting another preffix 'cyclo' before the word root. The suffix ane, ene or yne are written accordingly to the saturation or unsaturation in the ring structure. Some of the examples are.



Cyclo hexane

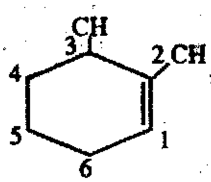


Cyclo pentene

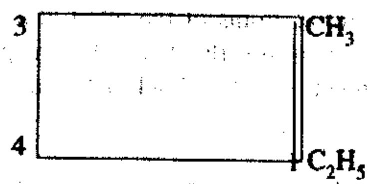


Cyclo pentyne

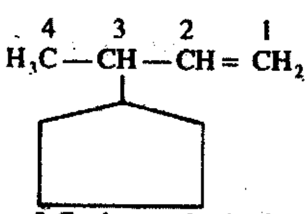
If some substituent is present, it is indicated by some appropriate prefix or suffix and its position is indicated by numbering the carbon atoms of the ring. The numbering is done in such a way so as to assign the least possible number to the substituent. Some examples are:



2,3 Dimethyl cyclo hexane



1 - Ethyl-2-methyl cyclo-butene

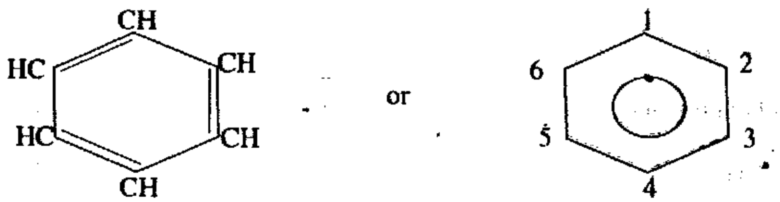


3-Cyclopentyl – 1 – butene

b) Naming the Aromatic compounds:

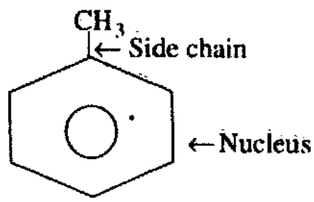
These compounds are cyclic compounds having double bond at alternate positions. Strictly speaking the position of double bond is not fixed at a point but changes all the time, hence double bonds are delocalised in these compounds.

The most important members of this class are benzene and its derivatives.

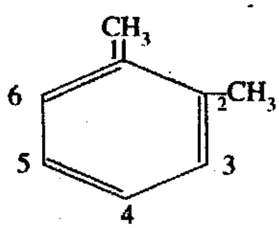


Benzene

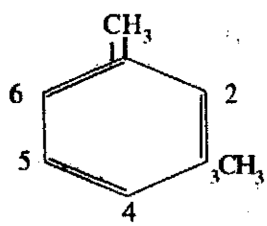
The carbon atoms of benzene are numbered from 1 to 6 as shown above. The benzene ring is called nucleus and alkyl groups like CH_3,CH_2CH_3 attached to nucleus are called side chains. This can be shown as



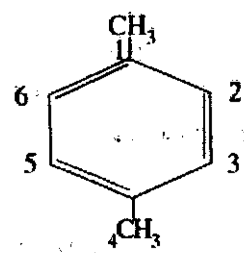
Benzene forms only one mono substituted derivative. It can form three disubstituted derivatives namely 1,2;1,3 and 1,4. These are called ortho (or O–) meta (or m–) and para (or p–) respectively



1,2 or ortho



1,3 or meta



1,4, or para

5.5 WRITING STRUCTURE OF HYDROCARBONS FROM IUPAC NAMES

Till now, we have named hydrocarbons from their structures using IUPAC nomenclature. Can we do reverse excercise? The reverse excercise i.e. writing structure of hydrocarbons when their IUPAC names are given. This excercise will confirm our ideas for naming organic compounds systematically. Let us take some examples to do this excercise.

Write the structure of

i) 4–ethyl–5–methyl–2–hexene

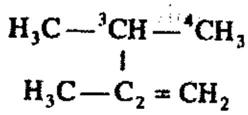
Ans. (carbons numbered 1 to 6)

$$\overset{1}{CH_3}-\overset{2}{CH}=\overset{3}{CH}-\underset{\displaystyle C_2H_5}{\overset{4}{CH}}-\underset{\displaystyle CH_3}{\overset{5}{CH}}.\overset{6}{CH_3}$$

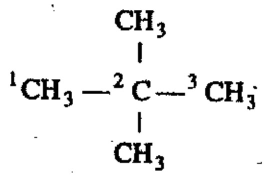
ii) 3,5 Octadiene

$$\overset{8}{CH_3}-\overset{7}{CH_2}-\overset{6}{CH}=\overset{5}{CH}-\overset{4}{CH}=\overset{3}{CH}-\overset{2}{CH_2}-\overset{1}{CH_3}$$

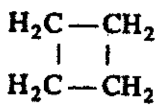
iii) 2.3 Dimethyl-1-butene



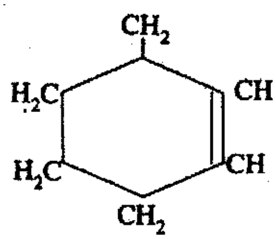
iv) 2,2— Dimethyl propane



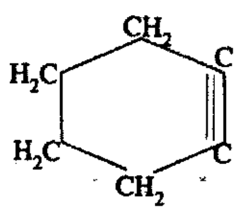
v) Cyclobutane



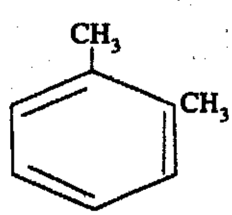
vi) Cyclohexene



vii) Cyclohexyn



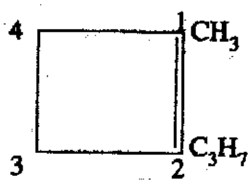
viii) 1,2 dimethyl Benzen



After this reverse excercise, you would have definitely gained confidance to name and write structure of all types of hydrocarbons.

NTEXT QUESTIONS 25.3

Write the name of the compound



....

Why did you number propyl as 2 in the answer of above question.

....

What do you mean by nucleus and side chain.

....

'5.6 WHAT YOU HAVE LEARNT

Hydrocarbons are the compounds of carbon and hydrogen.

Hydrocarbons are classified broadly into two categories i.e. open chain (acyclic) and closed chain (cyclic)

The open chain (acyclic) hydrocarbon contain alkanes, alkenes and alkynes.

The closed chain hydrocarbons contain alicyclic compounds like cyclo alkyne and aromatic compunds like benzene, toluene.

Importance of naming hydrocarbons using IUPAC system.

Important rules i.e. longest chain and lowest numbers to name hydrocarbons using IUPAC system.

Writing the names of hydrocarbons (open chain alicyclic and aromatic) using IUPAC system.

Writing structures of hydrocarbons from their IUPAC names.

.7 TERMINAL EXCERCISE

What do you mean by hydrocarbons? Give two examples.

....

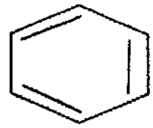
Why is benzene called an aromatic hydrocarbon. Give two examples of aromatic hydrocarbons.

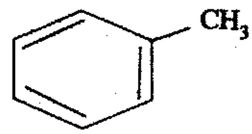
....

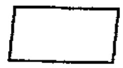
Classify the following hydrocarbons and write their names

i) $(CH_3)_3CH$ ii) $CH_3CH=CH_2$ iii) $(CH_3)_4C$

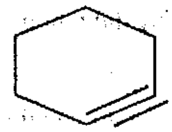
iv) $CH_3C\equiv CH$ v) $CH_3C\equiv CCH_3$ vi) $CH_2=CH_2$

vii)


viii)


ix)


x)


xi)


....

4. Write the possible structures and names of the following

i) C_5H_{10} ii) C_5H_8

....

5. Write the structures for the following compounds:

i) Isobutyl benzene ii) 4-methyl -2- pentyne.

iii) 1,6-heptadiene iv) Cyclobutene.

....

CHECK YOUR ANSWERS

INTEXT QUESTION 25.1

1. Alkane, alkene and alkyne

2. i) Cyclopentane ii) benzene

INTEXT QUESTIONS 25.2

1. i) Hexane

   ii) Pentene

   iii) Propyne

2. Longest chain rule and lowest number rule.

3. The sequence used is-position of substituent, name of the substituent, word root, suffix

INTEXT QUESTIONS 25.3

1. 1 - Methyl 2 - Propyl Cylobutene
2. The alphabatical letter P of propyl comes after M of Methyl.
3. Nucleus is the benzene ring and alkyl group attached to nucleus is called side chain.

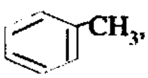
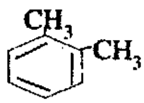
TERMINAL EXCERCISE

1. The compounds which are made up of carbon and hydrogen elements are known as hydrocarbons

   Examples: C_3H_8(Propane), C_6H_{12} (Hexene)

2. The name aromatic is derived from the Greek word 'aroma' meaning sweet smell.

   Benzene is the first member of this class and has sweet smell.

   Examples: , 

3.

	Classification	Names
i)	acyclic, saturated, alkane	2 methylpropane
ii)	acyclic, unsaturated, alkene	propene
iii)	acyclic saturated, alkane	2,2-dimethyl propane
iv)	acyclic, unsaturated, alkyne	Propyne
v)	acyclic, unsaturated, alkyne	2-butyne
vi)	acyclic, unsaturated, alkene	ethene
vii)	cyclic, arene	Benzene
viii)	cyclic, arene	Tolune
ix)	alicyclic, cyclo alkane	cyclobutane
x)	alicyclic, cycloalkene	cyclopentene
xi)	alicyclic cycloalkyne	cyclopentyne

4. (i) C_5H_{10}

   (a) $CH_3—CH_2—CH_2—CH=CH_2$ 1–pentene

   b) $CH_3CH_2—CH=CH—CH_3$ 2–Pentene

   c) $H_2C=C(CH_3)—CH_2—CH_3$ 2-methyl 1–butene

   d) $H_3C—C(CH_3)=CH—CH_3$ 2-methyl–2-butene

e)  Cyclo pentane

f) $CH_3-CH(CH_3)-CH=CH_2$
3-methyl-1-butene

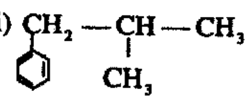
ii) C_5H_8

(a) $H_3C-CH_2-CH_2-C\equiv CH$
1-pentyne

(b) $H_3C-CH_2-C\equiv C-CH_3$
2-pentyne

(c) $H_3C-CH(CH_3)-C\equiv CH$
3-methyl-1-butyne

(d) 
cyclopentene

5. (i) 

(ii) $H_3C-C\equiv C-CH(CH_3)-CH_3$

(iii) $CH_2=CH-CH_2-CH_2-CH_2-CH=CH_2$

(iv)