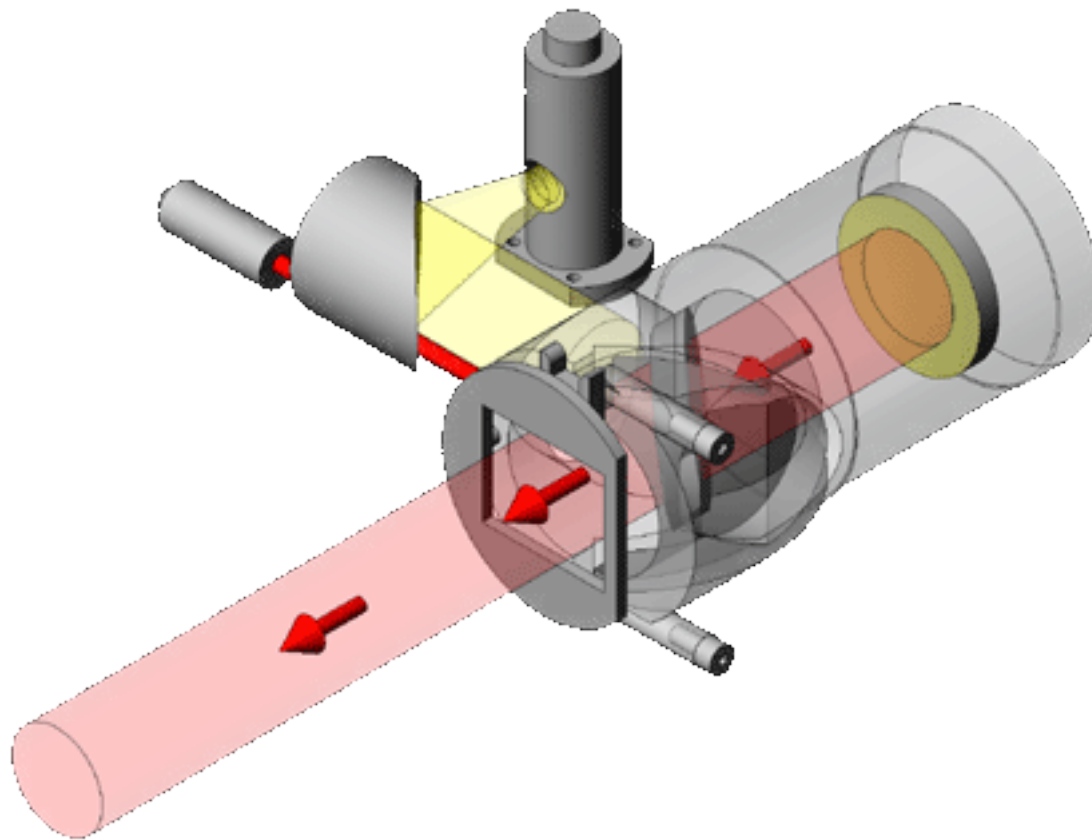

CHAPTER

1

BASIC CONCEPTS



Animation 1.1: Spectrometer
Source & Credit: gascell

1.1 ATOM

Long time ago, it was thought that matter is made up of simple, indivisible particles. Greek philosophers thought that, matter could be divided into smaller and smaller particles to reach a basic unit, which could not be further sub-divided. Democritus (460-370 B.C.) called these particles atomos, derived from the word “atomos” means indivisible. However, the ideas of Greek philosophers were not based on experimental evidences.

In the late 17th century, the quantitative study of the composition of pure substances disclosed that a few elements were the components of many different substances. It was also investigated that how, elements combined to form compounds and how compounds could be broken down into their constituent elements.

In 1808, an English school teacher, John Dalton, recognized that the law of conservation of matter and the law of definite proportions could be explained by the existence of atoms. He developed an atomic theory; the main postulate of which is that all matter is composed of atoms of different elements, which differ in their properties.

Atom is the smallest particle of an element, which can take part in a chemical reaction. For example, He and Ne, etc. have atoms, which have independent existence while atoms of hydrogen, nitrogen and oxygen do not exist independently.



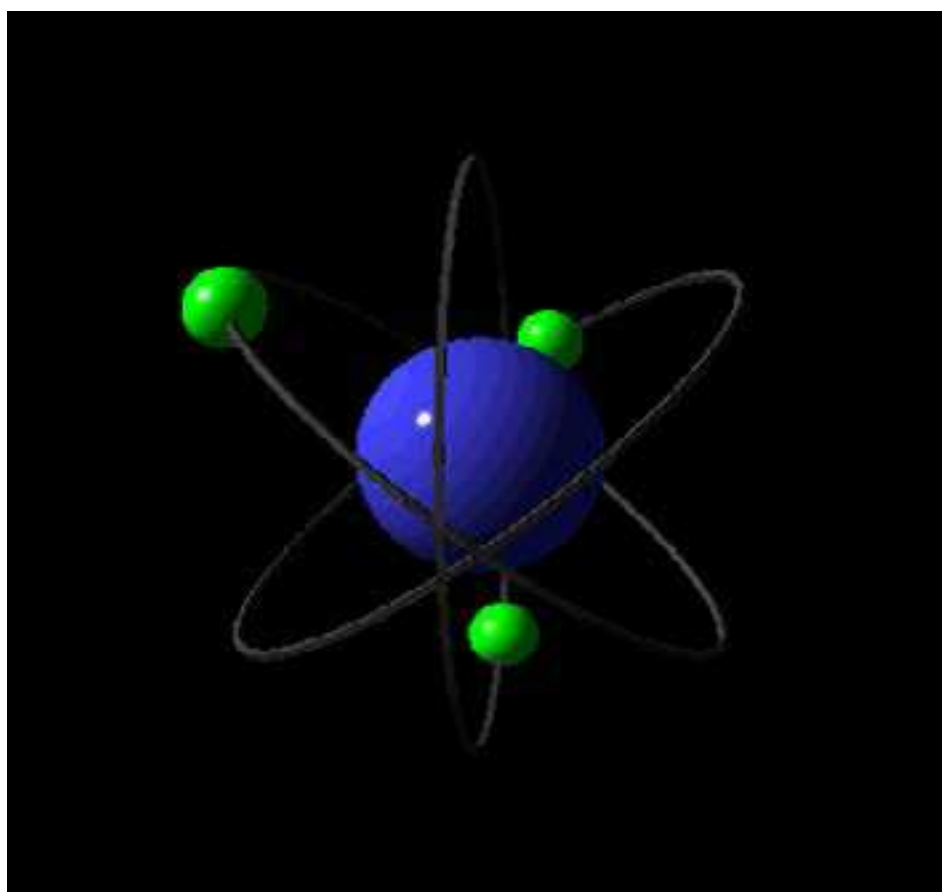
Animation 1.2: Atom
Source & Credit: 123gifs

The modern researches have clearly shown that an atom is further composed of subatomic particles like electron, proton, neutron, hyperon, neutrino, anti-neutrino, etc. More than 100 such particles are thought to exist in an atom. However, electron, proton and neutron are regarded as the fundamental particles of atoms.

A Swedish chemist J. Berzelius- (1779-1848) determined the atomic masses of elements. A number of his values are close to the modern values of atomic masses. Berzelius also developed the system of giving element a symbol.

1.1.1 Evidence of Atoms

It is not possible actually to see the atoms but the nearest possibility to its direct evidence is by using an electron microscope. A clear and accurate image of an object that is smaller than the wavelength of visible light, cannot be obtained. Thus an ordinary optical microscope can measure the size of an object upto or above 500 nm ($1\text{nm} = 10^{-9}\text{m}$). However, objects of the size of an atom can be observed in an electron microscope. It uses beams of electrons instead of visible light, because wavelength of electron is much shorter than that of visible light.



Animation 1.3:Made of Atom
Source & Credit: imgur

Fig. (1.1) shows electron microscopic photograph of a piece of a graphite which has been magnified about 15 millions times. The bright band in the figure are layers of carbon atoms.

In the 20th century, X-ray work has shown that the diameter of atoms are of the order 2×10^{-10} m which is 0.2 nm. Masses of atoms range from 10^{-27} to 10^{-25} kg. They are often expressed in atomic mass units (amu) when 1 amu is = 1.661×10^{-27} kg. The students can have an idea about the amazingly small size of an atom from the fact that a full stop may have two million atoms present in it.

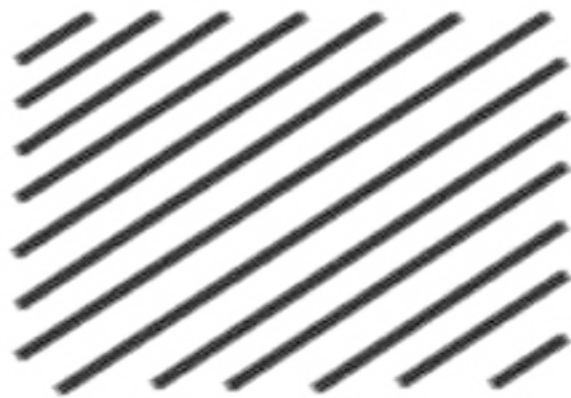


Fig (1.1) Electron microscopic photograph of graphite

1.1.2 Molecule

A molecule is the smallest particle of a pure substance which can exist independently. It may contain one or more atoms. The number of atoms present in a molecule determines its atomicity. Thus molecules can be monoatomic, diatomic and triatomic, etc., if they contain one, two and three atoms respectively. Molecules of elements may contain one, two or more same type of atoms. For example, He, Cl₂, O₃, P₄, S₈. On the other hand, molecules of compounds consist of different kind of atoms. For example, HCl, NH₃, H₂SO₄, C₆H₁₂O₆.

The sizes of molecules are definitely bigger than atoms. They depend upon the number of atoms present in them and their shapes. Some molecules are so big that they are called macromolecules. Haemoglobin is such a macromolecule found in blood. It helps to carry oxygen from our lungs to all parts of our body. Each molecule of haemoglobin is made up of nearly 10,000 atoms and it is 68,000 times heavier than a hydrogen atom.

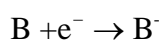
1.1.3 Ion

Ions are those species which carry either positive or negative charge. Whenever an atom of an element loses one or more electrons, positive ions are formed.

A sufficient amount of energy is to be provided to a neutral atom to ionize it.



This A^+ is called a cation. A cation may carry +1, +2, +3, etc. charge or charges. The number of charges present on an ion depends upon the number of electrons lost by the atom. Anyhow, energy is always required to do so. Hence the formation of the positive ions is an endothermic process. The most common positive ions are formed by the metal atoms such as Na^+ , K^+ , Ca^{2+} , Mg^{2+} , Al^{3+} , Fe^{3+} , Sn^{4+} , etc. The chapter on chemical bonding will enable us to understand the feasibilities of their formation. When a neutral atom picks up one or more electrons, a negative ion is produced, which is called an anion.

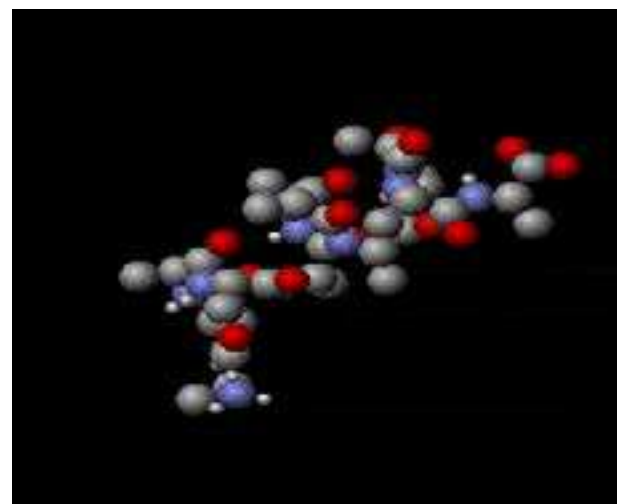


Energy is usually released when an electron is added to the isolated neutral atom, Therefore, the formation of an uninegative ion is an exothermic process. The most common negative ions are F^- , Cl^- , Br^- , S^{2-} etc.

The cations and anions possess altogether different properties from their corresponding neutral atoms. There are many examples of negative ions which consist of group of atoms like OH^- , CO_3^{2-} , SO_4^{2-} , PO_4^{3-} , MnO_4^{1-} , $Cr_2O_7^{2-}$ etc. The positive ions having group of atoms are less common e.g. NH_4^+ and some carbocations in organic chemistry.

1.1.4 Molecular Ion

When an atom loses or gains an electron, it forms an ion. Similarly, a molecule may also lose or gain an electron to form a molecular ion, e.g., CH_4^+ , CO^+ , N_2^+ Cationic molecular ions are more abundant than anionic ones. These ions can be generated by passing high energy electron beam or α -particles or X-rays through a gas. The break down of molecular ions obtained from the natural products can give important information about their structure.



Animation 1.4: Molecules
Source & credit: wikimedia

1.2 RELATIVE ATOMIC MASS

Relative atomic mass is the mass of an atom of an element as compared to the mass of an atom of carbon taken as 12.

The unit used to express the relative atomic mass is called atomic mass unit (amu) and it is $1/12$ th of the mass of one carbon atom, On carbon -12 scale, the relative atomic mass of $^{12}_6\text{C}$ is 12.0000 amu and the relative atomic mass of ^1_1H is 1.008 amu. The masses of the atoms are extremely small. We don't have any balance to weigh such an extremely small mass, that is why we use the relative atomic mass unit scale.

The relative atomic masses of some elements are given in the following Table (1.1).

Table (1.1) Relative atomic masses of a few elements

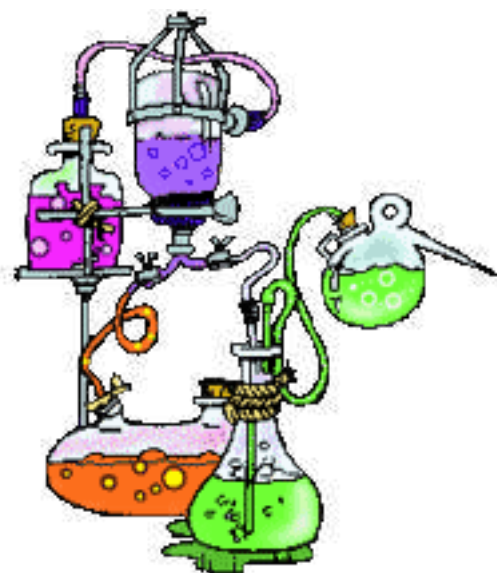
Element	Relative Atomic Mass (amu)	Element	Relative Atomic Mass (amu)
H	1.008	Cl	35.453
O	15.9994	Cu	63.546
Ne	20.1797	U	238.0289

These element have atomic masses in fractions and will be explained in the following article on isotopes.

1.3 ISOTOPES

In Dalton's atomic theory, all the atoms of an element were considered alike in all the properties including their masses. Later on, it was discovered that **atoms of the same element can possess different masses but same atomic numbers. Such atoms of an element are called isotopes.** So isotopes are different kind of atoms of the same element having same atomic number, but different atomic masses. The isotopes of an element possess same chemical properties and same position in the periodic table. This phenomenon of isotopy was first discovered by Soddy. Isotopes have same number of protons and electrons but they differ in the number of neutrons present in their nuclei.

Carbon has three isotopes written as $^{12}_6\text{C}$, $^{13}_6\text{C}$, $^{14}_6\text{C}$ and expressed as C-12, C-13 and C-14. Each of these have 6-protons and 6 electrons. However, these isotopes have 6, 7 and 8 neutrons respectively. Similarly, hydrogen has three isotopes ^1_1H , ^2_1H , ^3_1H called protium, deuterium and tritium. Oxygen has three, nickel has five, calcium has six, palladium has six, cadmium has nine and tin has eleven isotopes.



Animation 1.5: Basic Concepts
Source & Credit: pixshark

1.3.1 Relative Abundance of Isotopes

The isotopes of all the elements have their own natural abundance. The properties of a particular element, which are mentioned in the literature, mostly correspond to the most abundant isotope of that element. The relative abundance of the isotopes of elements can be determined by mass spectrometry.

Table (1.2) shows the natural abundance of some common isotopes.

Table (1.2) Natural abundance of some common isotopes.

Element	Isotope	Abundance (%)	Mass (amu)
Hydrogen	^1H , ^2H	99.985, 0.015	1.007825, 2.01410
Carbon	^{12}C , ^{13}C	98.893, 1.107	12.0000, 13.00335
Nitrogen	^{14}N , ^{15}N	99.634, 0.366	14.00307, 15.00011
Oxygen	^{16}O , ^{17}O , ^{18}O	99.759, 0.037, 0.204	15.99491, 16.99914, 17.9916
Sulphur	^{32}S , ^{33}S , ^{34}S , ^{36}S	95.0, 0.76, 4.22, 0.014	31.97207, 32.97146, 33.96786, 35.96709
Chlorine	^{36}Cl , ^{37}Cl	75.53, 24.47	34.96885, 36.96590
Bromine	^{79}Br , ^{81}Br	50.54, 49.49	78.918, 80.916

We know at present above 280 different isotopes occur in nature. They include 40 radioactive isotopes as well. Besides these about 300 unstable radioactive isotopes have been produced through artificial disintegration. The distribution of isotopes among the elements is varied and complex as it is evident from the Table (1.2). The elements like arsenic, fluorine, iodine and gold, etc have only a single isotope. They are called mono-isotopic elements.

In general, the elements of odd atomic number almost never possess more than two stable isotopes. The elements of even atomic number usually have larger number of isotopes and isotopes whose mass numbers are multiples of four are particularly abundant. For example, ^{16}O , ^{24}Mg , ^{28}Si , ^{40}Ca and ^{56}Fe form nearly 50% of the earth's crust. Out of 280 isotopes that occur in nature, 154 have even mass number and even atomic number.

1.3.2 Determination of Relative Atomic Masses of Isotopes by Mass Spectrometry

Mass spectrometer is an instrument which is used to measure the exact masses of different isotopes of an element. In this technique, a substance is first volatilized and then ionized with the help of high energy beam of electrons. The gaseous positive ions, thus formed, are separated on the basis of their mass to charge ratio (m/e) and then recorded in the form of peaks. Actually mass spectrum is the plot of data in such a way that (m/e) is plotted as abscissa (x-axis) and the relative number of ions as ordinate (y-axis).

First of all, Aston's mass spectrograph was designed to identify the isotopes of an element on the basis of their atomic masses. There is another instrument called Dempster's mass spectrometer. This was designed for the identification of elements which were available in solid state.

The substance whose analysis for the separation of isotopes is required, is converted into the vapour state. The pressure of these vapours is kept very low, that is, 10^{-6} to 10^{-7} torr. These vapours are allowed to enter the ionization chamber where fast moving electrons are thrown upon them. The atoms of isotopic element present in the form of vapours, are ionized. These positively charged ions of isotopes of an element have different masses depending upon the nature of the isotopes present in them.

The positive ion of each isotope has its own (m/e) value. When a potential difference (E) of 500-2000 volts is applied between perforated accelerating plates, then these positive ions are strongly attracted towards the negative plate. In this way, the ions are accelerated.

These ions are then allowed to pass through a strong magnetic field of strength (H), which will separate them on the basis of their (m/e) values. Actually, the magnetic field makes the ions to move in a circular path. The ions of definite m/e value will move in the form of groups one after the other and fall on the electrometer.

The mathematical relationship for (m/e) is

$$m/e = H^2 r / 2E$$

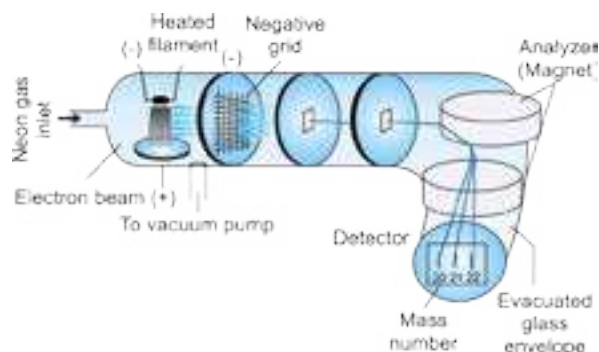
Where H is the strength of magnetic field, E is the strength of electrical field, r is the radius of circular path. If E is increased, by keeping H constant then radius will increase and positive ion of a particular m/e will fall at a different place as compared to the first place. This can also be done by changing the magnetic field. Each ion sets up a minute electrical current.

Electrometer is also called an ion collector and develops the electrical current. The strength of the current thus measured gives the relative abundance of ions of a definite m/e value.

Similarly, the ions of other isotopes having different masses are made to fall on the collector and the current strength is measured. The current strength in each case gives the relative abundance of each of the isotopes. The same experiment is performed with C-12 isotope and the current strength is compared.

This comparison allows us to measure the exact mass number of the isotope Fig. (1.2), shows the separation of isotopes of Ne. Smaller the (m/e) of an isotope, smaller the radius of curvature produced by the magnetic field according to above equation.

In modern spectrographs, each ion strikes a detector, the ionic current is amplified and is fed to the recorder. The recorder makes a graph showing the relative abundance of isotopes plotted against the mass number.



Fig(1.2) Diagram of a simple Mass Spectrometer

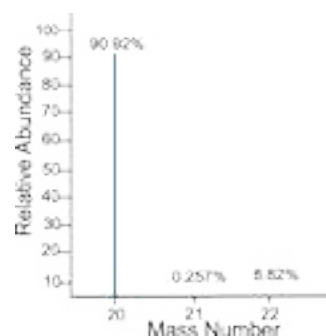


Fig (1.3) Computer plotted graph for the isotopes of neon

The above Fig (1.3) shows a computer plotted graph for the isotopes of neon.

The separation of isotopes can be done by the methods based on their properties. Some important methods are as gaseous diffusion, thermal diffusion, distillation, ultracentrifuge, electromagnetic separation and laser separation.

1.3.3 Average Atomic Masses

Table (1.1) of atomic masses of elements shows many examples of fractional values. Actually the atomic masses depend upon the number of possible isotopes and their natural abundance. Following solved example will throw light on this aspect.

Example (1):

A sample of neon is found to consist of $^{20}_{10}\text{Ne}$, $^{21}_{10}\text{Ne}$ and $^{22}_{10}\text{Ne}$ in the percentages of 90.92%, 0.26%, 8.82% respectively. Calculate the fractional atomic mass of neon.

Solution:

The overall atomic mass of neon, which is an ordinary isotopic mixture, is the average of the determined atomic masses of individual isotopes. Hence

$$\text{Average atomic mass} = \frac{20 \times 90.92 + 21 \times 0.26 + 22 \times 8.82}{100} = 20.18 \text{ Answer}$$

Hence the average atomic mass of neon is 20.18 amu

It is important to realize that no individual neon atom in the sample has a mass of 20.18 amu. For most laboratory purposes, however, we consider the sample to consist of atoms with this average mass.

1.4 ANALYSIS OF A COMPOUND - EMPIRICAL AND MOLECULAR FORMULAS

Before we go into the details of empirical and molecular formulas of a compound, we should be interested to know the percentage of each element in the compound. For this purpose all the elements present in the compound are first identified.

This is called qualitative analysis. After that the compound is subjected to quantitative analysis in which the mass of each element in a sample of the compound is determined. From this we determine the percentage by mass of each element. The percentage of an element in a compound is the number of grams of that element present in 100 grams of the compound.

$$\text{Percentage of an element} = \frac{\text{Mass of the element in the compound}}{\text{mass of the compound}} \times 100$$

Example (2):

8.657 g of a compound were decomposed into its elements and gave 5.217 g of carbon, 0.962 g of hydrogen, 2.478 g of oxygen. Calculate the percentage composition of the compound under study.

Solution:

Applying the formula

$$\text{Percentage of carbon} = \frac{\text{Mass of carbon}}{\text{Mass of the compound}} \times 100 = \frac{5.217g}{8.657g} \times 100 = 60.28 \text{ Answer}$$

$$\text{Percentage of hydrogen} = \frac{\text{Mass of hydrogen}}{\text{Mass of the compound}} \times 100 = \frac{0.962g}{8.657g} \times 100 = 11.11 \text{ Answer}$$

$$\text{Percentage of oxygen} = \frac{\text{Mass of oxygen}}{\text{Mass of the compound}} \times 100 = \frac{2.478g}{8.657g} \times 100 = 28.62 \text{ Answer}$$

The above results tell us that in one hundred grams of the given compound, there are 60.26 grams of carbon, 11.11 grams of hydrogen and 28.62 grams of oxygen.

Percentage composition of a compound can also be determined theoretically if we know the formula mass of the compound. The following equation can be used for this purpose.

$$\text{Percentage of an element} = \frac{\text{Mass of the element in one mole of the compound}}{\text{Formula mass of the compound}} \times 100$$

1.4.1 Empirical Formula

It is the simplest formula that gives the small whole number ratio between the atoms of different elements present in a compound. In an empirical formula of a compound, $A_x B_y$, there are x atoms of an element A and y atoms of an element B.

The empirical formula of glucose ($C_6H_{12}O_6$) is CH_2O and that of benzene (C_6H_6) is CH .

Empirical formula of a compound can be calculated following the steps mentioned below:

1. Determination of the percentage composition.
2. Finding the number of gram atoms of each element. For this purpose divide the mass of each element (% of an element) by its atomic mass.
3. Determination of the atomic ratio of each element. To get this, divide the number of moles of each element (gram atoms) by the smallest number of moles.
4. If the atomic ratio is simple whole number, it gives the empirical formula, otherwise multiply with a suitable digit to get the whole number atomic ratio.

Example (3):

Ascorbic acid (vitamin C) contains 40.92% carbon, 4.58% hydrogen and 54.5% of oxygen by mass. What is the empirical formula of the ascorbic acid?

Solution:

From the percentages of these elements, we believe that in 100 grams of ascorbic acid, there are 40.92 grams of carbon, 4.58 grams of hydrogen and 54.5 grams of oxygen.

Divide these masses of the elements (or percentages) by their atomic masses to get the number of gram atoms.

$$\text{No. of gram atoms of hydrogen} = \frac{4.58\text{g}}{1.008 \text{ gmol}^{-1}} = 4.54 \text{ gram atoms}$$

$$\text{No. of gram atoms of oxygen} = \frac{54.5\text{g}}{16 \text{ gmol}^{-1}} = 3.406 \text{ gram atoms}$$

$$\text{No. of gram atoms of carbon} = \frac{40.92\text{g}}{12.0 \text{ gmol}^{-1}} = 3.41 \text{ gram atoms}$$

Atomic ratio is obtained by dividing the gram atoms with 3.406, which is the smallest number.

$$\text{C:H:O} = \frac{3.41}{3.406} : \frac{4.54}{3.406} : \frac{3.406}{3.406}$$

$$\text{C:H:O} = 1 : 1.33 : 1$$

To convert them into whole numbers, multiply with three

$$\text{C:H:O} = 3(1 : 1.33 : 1) = \boxed{3 : 4 : 3} \text{ Answer}$$

This whole number ratio gives us the subscripts for the empirical formula of the ascorbic acid i.e., $\text{C}_3\text{H}_4\text{O}_3$.

1.4.2 Empirical Formula from Combustion Analysis

Those organic compounds which simply consist of carbon, hydrogen and oxygen can be analyzed by combustion. The sole products will be CO_2 and H_2O . These two products of combustion are separately collected.

Combustion Analysis

A weighed sample of the organic compound is placed in the combustion tube. This combustion tube is fitted in a furnace. Oxygen is supplied to burn the compound. Hydrogen is converted to H_2O and carbon is converted to CO_2 . These gases are absorbed in $\text{Mg}(\text{ClO}_4)_2$ and 50% KOH respectively. (Fig 1.4). The difference in the masses of these absorbers gives us the amounts of H_2O and CO_2 produced. The amount of oxygen is determined by the method of difference.



Fig(1.4) Combustion analysis

Following formulas are used to get the percentages of carbon, hydrogen and oxygen, respectively.

$$\% \text{ of carbon} = \frac{\text{Mass of } \text{CO}_2}{\text{Mass of organic compound}} \times \frac{12.00}{44.00} \times 100$$

$$\% \text{ of hydrogen} = \frac{\text{Mass of } \text{H}_2\text{O}}{\text{Mass of organic compound}} \times \frac{2.016}{18} \times 100$$

The percentage of oxygen is obtained by the method of difference.

$$\% \text{ of oxygen} = 100 - (\% \text{ of carbon} + \% \text{ of hydrogen}).$$

Example (4):

A sample of liquid consisting of carbon, hydrogen and oxygen was subjected to combustion analysis. 0.5439 g of the compound gave 1.039 g of CO_2 , 0.6369 g of H_2O . Determine the empirical formula of the compound.

Solution:

Mass of organic Compound	= 0.5439 g
Mass of carbon dioxide	= 1.039g
Mass of water	= 0.6369 g

Element	%	No. of Gram atoms	Atomic Ratio	Empirical formula
C	$\frac{1.039\text{g}}{0.543\text{g}} \times \frac{12.00}{44.00} \times 100$ =52.108	$\frac{52.108}{12} = 4.34$	$\frac{4.34}{2.17} = 2$	C ₂ H ₆ O
H	$\frac{0.6369\text{g}}{0.5439\text{g}} \times \frac{2.016}{18} \times 100$ =13.11	$\frac{13.11}{1.008} = 13.01$	$\frac{13.01}{2.17} = 6$	
O	$100 - (52.108 + 13.11)$ =34.77	$\frac{34.77}{16.00} = 2.17$	$\frac{2.17}{2.17} = 1$	

1.4.3 Molecular Formula

That formula of a substance which is based on the actual molecule is called molecular formula. It gives the total number of atoms of different elements present in the molecule of a compound. For example, molecular formula of benzene is C₆H₆ while that of glucose is C₆H₁₂O₆.

The empirical formulas of benzene and glucose are CH and CH₂O respectively, so for these compounds the molecular formulas are the simple multiple of empirical formulas. Hence

$$\text{Molecular formula} = n (\text{Empirical formula})$$

Where 'n' is a simple integer. Those compounds whose empirical and molecular formulae are the same are numerous. For example, H₂O, CO₂, NH₃ and C₁₂H₂₂O₁₁ have same empirical and molecular formulas. Their simple multiple 'n' is unity. Actually the value of 'n' is the ratio of molecular mass and empirical formula mass of a substance.

$$n = \frac{\text{Molecular mass}}{\text{Empirical formula mass}}$$

Example (5):

The combustion analysis of an organic compound shows it to contain 65.44% carbon, 5.50% hydrogen and 29.06% oxygen. What is the empirical formula of the compound? If the molecular mass of this compound is $110.15 \text{ g.mol}^{-1}$. Calculate the molecular formula of the compound.

Solution:

First of all divide the percentage of each element by its atomic mass to get the number of gram atoms or moles.

$$\text{No of gram atoms of C} = \frac{65.44 \text{ g of C}}{12 \text{ g / mol}} = 5.45 \text{ gram atoms of C}$$

$$\text{No of gram atoms of hydrogen} = \frac{5.50 \text{ g of H}}{1.008 \text{ g / mol}} = 5.46 \text{ gram atoms of H}$$

$$\text{No of gram atoms of oxygen} = \frac{29.06 \text{ g of O}}{16.00 \text{ g / mol}} = 1.82 \text{ gram atoms of O}$$

Molar ratio:

$$\begin{array}{ccccccc} \text{C} & : & \text{H} & : & \text{O} & & \\ 5.45 & : & 4.46 & : & 1.82 & & \end{array}$$

Divide the number of gram atoms by the smallest number i.e 1.82

$$\begin{array}{ccccccc} \text{C} & : & \text{H} & : & \text{O} & & \\ \frac{5.45}{1.82} & : & \frac{5.46}{1.82} & : & \frac{1.82}{1.82} & & \\ 3 & : & 3 & : & 1 & & \end{array}$$

Carbon, hydrogen and oxygen are present in the given organic compound in the ratio of 3:3:1. So the empirical formula is $\text{C}_3\text{H}_3\text{O}$.

In order to determine the molecular formula, first calculate the empirical formula mass.

$$\text{Empirical formula mass} = 12 \times 3 + 1.008 \times 3 + 16 \times 1 = 55.05 \text{ g/mol}$$

$$\text{Molar mass of the compound} = 110.15 \text{ g.mol}^{-1}$$

$$n = \frac{\text{Molar mass of the compound}}{\text{Empirical formula mass}} = \frac{110.15}{55.05} = 2$$

$$\begin{aligned} \text{Molecular formula} &= n (\text{empirical formula}) \\ &= 2 (\text{C}_3\text{H}_3\text{O}) = \text{C}_6\text{H}_6\text{O}_2 \text{ Answer} \end{aligned}$$

There are many possible structures for this molecular formula.

1.5 CONCEPT OF MOLE

We know that atom is an extremely small particle. The mass of an individual atom is extremely small quantity. It is not possible to weigh individual atoms or even small number of atoms directly. That is why, we use the atomic mass unit (amu) to express the atomic masses.

For the sake of convenience, the atomic mass may be given in any unit of measurement i.e. grams, kg, pounds, and so on.

When the substance at our disposal is an element then the atomic mass of that element expressed in grams is called one gram atom. It is also called one gram mole or simply a mole of that element.

$$\text{Number of gram atoms or moles of an element} = \frac{\text{Mass of an element in grams}}{\text{Molar mass of an element}}$$

For example

$$\begin{aligned} 1 \text{ gram atom of hydrogen} &= 1.008 \text{ g} \\ 1 \text{ gram atom of carbon} &= 12.000 \text{ g} \\ \text{and } 1 \text{ gram atom of uranium} &= 238.0 \text{ g} \end{aligned}$$

It means that one gram atom of different elements have different masses in them. One mole of carbon is 12 g, while 1 mole of magnesium is 24g. It also shows that one atom of magnesium is twice as heavy as an atom of carbon.

The molecular mass of a substance expressed in grams is called gram molecule or gram mole or simply the mole of a substance.

$$\text{Number of gram molecules or moles of a molecular substance} = \frac{\text{Mass of molecular substance in grams}}{\text{Molar mass of the substance}}$$

For example

$$\begin{array}{l} 1 \text{ gram molecule of water} = 18.0 \text{ g} \\ 1 \text{ gram molecule of H}_2\text{SO}_4 = 98.0 \text{ g} \\ \text{and } 1 \text{ gram molecule of sucrose} = 342.0 \text{ g} \end{array}$$

It means that one gram molecules of different molecular substances have different masses.

The formula unit mass of an ionic compound expressed in grams is called gram formula of the substance. Since ionic compounds do not exist in molecular form therefore the sum of atomic masses of individual ions gives the formula mass. The gram formula is also referred to as gram mole or simply a mole.

$$\text{Number of gram formulas or moles of a substance} = \frac{\text{Mass of the ionic substance in grams}}{\text{Formula mass of the ionic substance}}$$

$$\begin{array}{l} 1 \text{ gram formula of NaCl} = 58.50 \text{ g} \\ 1 \text{ gram formula of Na}_2\text{CO}_3 = 106 \text{ g} \\ 1 \text{ gram formula of AgNO}_3 = 170 \text{ g} \end{array}$$

It may also be mentioned here that ionic mass of an ionic species expressed in grams is called one gram ion or one mole of ions.

$$\text{Number of gram ions or moles of an species} = \frac{\text{Mass of the ionic species in grams}}{\text{Formula mass of the ionic species}}$$

For example

$$\begin{array}{l} 1 \text{ g ion of OH}^- = 17 \text{ g} \\ 1 \text{ g ion of SO}_4^{2-} = 96 \text{ g} \\ 1 \text{ g ion of CO}_3^{2-} = 60 \text{ g} \end{array}$$

So, the atomic mass, molecular mass, formula mass or ionic mass of the substance expressed in gram is called molar mass of the substance.

Example (6):

Calculate the gram atoms (moles) in

- (a) 0.1 g of sodium.
 (b) 0.1 kg of silicon.

Solution

$$(a) \text{ No. of gram atoms} = \frac{\text{Mass of element in gram}}{\text{Molar mass}}$$

$$\begin{aligned} \text{Mass of sodium} &= 0.1 \text{ g} \\ \text{Molar mass} &= 23 \text{ g/mol} \end{aligned}$$

$$\text{Number of gram atoms of sodium} = \frac{0.1 \text{ g}}{23 \text{ gmol}^{-1}} = 0.0043 \text{ mol}$$

$$= \boxed{4.3 \times 10^{-3} \text{ mol}} \quad \text{Answer}$$

(b) First of all convert the mass of silicon into grams.

$$\begin{aligned} \text{Mass of silicon} &= 0.1 \text{ kg} &= 0.1 \times 1000 = 100 \text{ g} \\ \text{Molar mass} &&= 28.086 \text{ gmol}^{-1} \end{aligned}$$

$$\text{Number of gram atoms of silicon} = \frac{100 \text{ g}}{28.086 \text{ gmol}^{-1}} = \boxed{3.56 \text{ moles}} \quad \text{Answer}$$

Example (7):

Calculate the mass of 10^{-3} moles of MgSO_4 .

Solution:

MgSO_4 is an ionic compound. We will consider its formula mass in place of molecular mass.

$$\text{Number of gram formula or mole of a substance} = \frac{\text{Mass of the ionic substance}}{\text{Formula mass of the ionic substance}}$$

Formula mass of $\text{MgSO}_4 = 24 + 96 = 120 \text{ gmol}^{-1}$

Number of moles of $\text{MgSO}_4 = 10^{-3}$ moles

Applying the formula

$$10^{-3} = \frac{\text{Mass of MgSO}_4}{120 \text{ gmol}^{-1}}$$

Mass of $\text{MgSO}_4 = 10^{-3}$ moles $\times 120 \text{ gmol}^{-1}$

$$= 120 \times 10^{-3} = \boxed{0.12 \text{ g}} \text{ Answer}$$

1.5.1 Avogadro's Number

Avogadro's number is the number of atoms, molecules and ions in one gram atom of an element, one gram molecule of a compound and one gram ion of a substance, respectively.

To understand Avogadro's number let us consider the following quantities of substances.

1.008 g of hydrogen = 1 mole of hydrogen = 6.02×10^{23} atoms of H

23 g of sodium = 1 mole of Na = 6.02×10^{23} atoms of Na

238 g of uranium = 1 mole of U = 6.02×10^{23} atoms of U

This number, 6.02×10^{23} is the number of atoms in one mole of the element. It is interesting to know that different masses of elements have the same number of atoms. An atom of sodium is 23 times heavier than an atom of hydrogen. In order to have equal number of atoms sodium should be taken 23 times greater in mass than hydrogen. Magnesium atom is twice heavier than carbon; i.e. 10 g of Mg and 5 g of C contain the same number of atoms.

18 g of H_2O = 1 mole of water = 6.02×10^{23} molecules of water

180 g of glucose = 1 mole of glucose = 6.02×10^{23} molecules of glucose

342 g of sucrose = 1 mole of sucrose = 6.02×10^{23} molecules of sucrose

Hence, one mole of different compounds has different masses but has the same number of molecules.

When we take into consideration the ions, then

96 g of SO_4^{2-} = 1 mole of SO_4^{2-} = 6.02×10^{23} ions of SO_4^{2-}

62 g of NO_3^- = 1 mole of NO_3^- = 6.02×10^{23} ions of NO_3^-

From the above discussion, we reach the conclusion that the number 6.02×10^{23} is equal to one mole of a substance. This number is called Avogadro's number and it is denoted by N_A . Following relationships between amounts of substances in terms of their masses and the number of particles present in them, are useful

$$1) \quad \text{Number of atoms of an element} = \frac{\text{Mass of the element} \times N_A}{\text{Atomic mass}}$$

$$2) \quad \text{Number of molecules of a compound} = \frac{\text{Mass of the compound} \times N_A}{\text{Molecular mass}}$$

$$3) \quad \text{Number of ions of an ionic species} = \frac{\text{Mass of the ion} \times N_A}{\text{Ionic mass}}$$

When we have compounds of known mass we can calculate the number of atoms from their formulas. In 18 g of water there are present 6.02×10^{23} molecules of H_2O , $2 \times 6.02 \times 10^{23}$ atoms of hydrogen and 6.02×10^{23} atoms of oxygen. Similarly, in 98g of H_2SO_4 , it has twice the Avogadro's number of hydrogen atoms, four times the Avogadro's number of oxygen atoms and the Avogadro's number of sulphur atoms.

Some substances ionize in suitable solvents to yield cations and anions. The number of such ions, their masses, number of positive and negative charges can be easily calculated from the known amount of the substance dissolved. Let us dissolve 9.8 g of H_2SO_4 in sufficient quantity of H_2O to get it completely ionized. It has 0.1 moles of H_2SO_4 . It will yield 0.2 mole or $0.2 \times 6.02 \times 10^{23}$ H^+ and 0.1 moles or $0.1 \times 6.02 \times 10^{23}$ SO_4^{2-} etc. Total positive charges will be $0.2 \times 6.02 \times 10^{23}$ and the total negative charges will be $0.2 \times 6.02 \times 10^{23}$ (because each SO_4^{2-} , has two negative charges). The total mass of H^+ is (0.2×1.008) g and that of SO_4^{2-} is (0.1×96) g.

Example (8):

How many molecules of water are there in 10.0 g of ice? Also calculate the number of atoms of hydrogen and oxygen separately, the total number of atoms and the covalent bonds present in the sample.

Solution:

$$\begin{aligned}\text{Mass of ice (water)} &= 10.0 \text{ g} \\ \text{Molar mass of water} &= 18 \text{ g mol}^{-1}\end{aligned}$$

$$\begin{aligned}\text{Number of molecules of water} &= \frac{\text{Mass of water in gram}}{\text{Molar mass of water in g mol}^{-1}} \times \text{Avogadro's number} \\ &= \frac{10}{18 \text{ g mol}^{-1}} \times 6.02 \times 10^{23}\end{aligned}$$

$$\begin{aligned}\text{Number of molecules of water} &= 0.55 \times 6.02 \times 10^{23} &&= \boxed{3.31 \times 10^{23}} \text{ Answer} \\ \text{One molecule of water contain hydrogen atoms} &&&= 2 \\ \text{3.31} \times 10^{23} \text{ molecules of water contain hydrogen atoms} &&&= 2 \times 3.31 \times 10^{23} \\ &&&= \boxed{6.68 \times 10^{23}} \text{ Answer} \\ \text{One molecule of water contains oxygen atom} &&&= 1 \\ \text{3.31} \times 10^{23} \text{ molecules of water contain oxygen atoms} &&&= \boxed{3.31 \times 10^{23}} \text{ Answer} \\ \text{One molecule of water contains number of covalent bonds} &&&= 2 \\ \text{3.31} \times 10^{23} \text{ molecules of water contain number of covalent bonds} &&&= 2 \times 3.31 \times 10^{23} \\ &&&= \boxed{6.68 \times 10^{23}} \text{ Answer} \\ \text{Total number of atoms of hydrogen and oxygen} &&&= 6.68 \times 10^{23} + 3.31 \times 10^{23} \\ &&&= \boxed{9.99 \times 10^{23}} \text{ Answer}\end{aligned}$$

Example (9):

10.0 g of H_3PO_4 has been dissolved in excess of water to dissociate it completely into ions. Calculate,

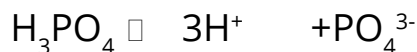
- Number of molecules in 10.0 g of H_3PO_4 .
- Number of positive and negative ions in case of complete dissociation in water.
- Masses of individual ions.
- Number of positive and negative charges dispersed in the solution.

Solution:

$$\begin{aligned}\text{(a)} \quad \text{Mass of } \text{H}_3\text{PO}_4 &= 10 \text{ g} \\ \text{Molar mass of } \text{H}_3\text{PO}_4 &= 3 + 31 + 64 = 98 \\ \text{No. of molecules of } \text{H}_3\text{PO}_4 &= \frac{\text{Mass of } \text{H}_3\text{PO}_4}{\text{Molar mass of } \text{H}_3\text{PO}_4} \times 6.02 \times 10^{23}\end{aligned}$$

$$\begin{aligned}
 &= \frac{10}{98 \text{ g mol}^{-1}} \times 6.02 \times 10^{23} \\
 &= 0.102 \times 6.02 \times 10^{23} \\
 &= 0.614 \times 10^{23} \\
 &= \boxed{6.14 \times 10^{22}} \text{ Answer}
 \end{aligned}$$

(b) H_3PO_4 dissolves in water and ionizes as follows



According to the balanced chemical equation

H_3PO_4	:	H^+
1	:	3
6.14×10^{22}	:	$3 \times 6.14 \times 10^{22}$
6.14×10^{22}	:	1.842×10^{23}

Hence, the number of H^+ will be 1.842×10^{23}

H_3PO_4	:	PO_4^{3-}
1	:	1
6.14×10^{22}	:	6.14×10^{22}

Hence, the number of PO_4^{3-} will be $\boxed{6.14 \times 10^{22}}$ Answer

(c) In order to calculate the mass of the ions, use the formulas

$$\text{Number of H}^+ = \frac{\text{Total mass of H}^+}{\text{Ionic mass of H}^+} \times 6.02 \times 10^{23}$$

$$1.842 \times 10^{23} = \frac{\text{Total mass of H}^+}{1.008} \times 6.02 \times 10^{23}$$

$$\text{Total mass of H}^+ = \frac{1.842 \times 10^{23} \times 1.008}{6.02 \times 10^{23}} = 0.308 \text{ g}$$

$$\text{No. of PO}_4^{3-} = \frac{\text{Total mass of PO}_4^{3-}}{\text{Ionic mass of PO}_4^{3-}} \times 6.02 \times 10^{23} \text{ molecules}$$

$$6.14 \times 10^{22} = \frac{\text{Total mass of PO}_4^{3-}}{95} \times 6.02 \times 10^{23}$$

$$\text{Total mass of PO}_4^{3-} = \frac{6.14 \times 10^{22} \times 95}{6.02 \times 10^{23}} = \boxed{9.689\text{g}} \text{ Answer}$$

(d) One molecule of H_3PO_4 gives three positive charges in the solution

$$6.14 \times 10^{22} \text{ molecules of } \text{H}_3\text{PO}_4 \text{ will give } = 3 \times 6.14 \times 10^{22}$$

$$= \boxed{1.842 \times 10^{23} \text{ positive charges}} \text{ Answer}$$

Number of positive and negative charges are always equal. So the number of negative charges dispersed in the solution = 1.842×10^{23}

1.5.2 Molar Volume

One mole of any gas at standard temperature and pressure (STP) occupies a volume of 22.414 dm³. This volume of 22.414 dm³ is called molar volume and it is true only when the gas is ideal (the idea of the ideality of the gas is mentioned in chapter three).

With the help of this information, we can convert the mass of a gas at STP into its volume and vice versa.

Hence we can say that

2.016 g of H₂ = 1 mole of H₂ = 6.02 × 10²³ molecules of H₂ = 22.414 dm³ of H₂ at S.T.P

16g of CH₄ = 1 mole of CH₄ = 6.02 × 10²³ molecules of CH₄ = 22.414 dm³ of CH₄ at S.T.P.

It is very interesting to know from the above data that 22.414 dm³ of each gas has a different mass but the same number of molecules. The reason is that the masses and the sizes of the molecules don't affect the volumes. Normally, it is known that in the gaseous state the distance between molecules is 300 times greater than their diameters.

Example (10):

A well known ideal gas is enclosed in a container having volume 500 cm³ at S.T.P. Its mass comes out to be 0.72g. What is the molar mass of this gas.

Solution:

We can calculate the number of moles of the ideal gas at S.T.P from the given volume.

22.414 dm³ or 22.414 cm³ of the ideal gas at S.T.P = 1 mole

$$1 \text{ cm}^3 \text{ of the ideal gas at S.T.P} = \frac{1}{22414} \text{ mole}$$

$$\begin{aligned} 500 \text{ cm}^3 \text{ of the ideal gas at S.T.P} &= \frac{1}{22414} \times 500 \\ &= 0.0223 \text{ moles} \end{aligned}$$

We know that

$$\text{Number of moles of the gas} = \frac{\text{Mass of the gas}}{\text{Molar mass of the gas}}$$

$$\text{Molar mass of the gas} = \frac{\text{Mass of the gas}}{\text{Number of moles of the gas}}$$

$$\text{Molar mass of the gas} = \frac{0.72 \text{ g}}{0.0223 \text{ mole}} = \boxed{32 \text{ g mol}^{-1}} \text{ Answer}$$

1.6 STOICHIOMETRY

With the knowledge of atomic mass, molecular mass, the mole, the Avogadro's number and the molar volume, we can make use of the chemical equations in a much better way and can get many useful information from them.

Chemical equations have certain limitations as well. They do not tell about the conditions and the rate of reaction. Chemical equation can even be written to describe a chemical change that does not occur. So, when stoichiometric calculations are performed, we have to assume the following conditions.

1. All the reactants are completely converted into the products.
2. No side reaction occurs.

Stoichiometry is a branch of chemistry which tells us the quantitative relationship between reactants and products in a balanced chemical equation.

While doing calculations, the law of conservation of mass and the law of definite proportions are obeyed.

The following type of relationships can be studied with the help of a balanced chemical equation.

1) Mass-mass Relationship

If we are given the mass of one substance, we can calculate the mass of the other substances involved in the chemical reaction.

2) Mass-mole Relationship or Mole-mass Relationship

If we are given the mass of one substance, we can calculate the moles of other substance and vice-versa.

3) Mass-volume Relationship

If we are given the mass of one substance, we can calculate the volume of the other substances and vice-versa. Similarly, mole-mole calculations can also be performed.

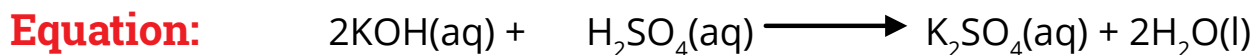
Example (11):

Calculate the number of grams of K_2SO_4 and water produced when 14 g of KOH are reacted with excess of H_2SO_4 . Also calculate the number of molecules of water produced.

Solution:

For doing such calculations, first of all convert the given mass of KOH into moles and then compare these moles with those of K_2SO_4 with the help of the balanced chemical equation.

$$\begin{aligned} \text{Mass of KOH} &= 14.0 \text{ g} \\ \text{Molar mass of KOH} &= 39 + 16 + 1 = 56 \text{ g/mol} \\ \text{Number of moles of KOH} &= \frac{14.0 \text{ g}}{56 \text{ g mol}^{-1}} = 0.25 \end{aligned}$$



To get the number of moles of K_2SO_4 , compare the moles of KOH with those of K_2SO_4 .

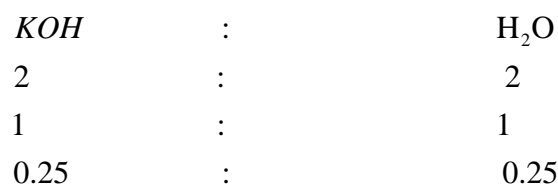
KOH	:	K_2SO_4
2	:	1
1	:	$\frac{1}{2}$
0.25	:	0.125

So, 0.125 moles of K_2SO_4 is being produced from 0.25 moles of KOH

$$\begin{aligned} \text{Molar mass of } K_2SO_4 &= 2 \times 39 + 96 \\ &= 174 \text{ g/mol} \end{aligned}$$

$$\begin{aligned} \text{Mass of } K_2SO_4 \text{ produced} &= \text{No. of moles} \times \text{molar mass} \\ &= 0.125 \text{ moles} \times 174 \text{ g mol}^{-1} \\ &= 21.75 \text{ g} \end{aligned}$$

To get the number of moles of H_2O , compare the moles of KOH with those of water



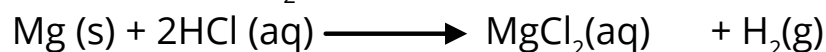
So, the number of moles of water produced is 0.25 from 0.25 moles of KOH

$$\begin{aligned}
 \text{Mass of water produced} &= 0.25 \text{ moles} \times 18 \text{ g mol}^{-1} \\
 &= 4.50 \text{ g}
 \end{aligned}$$

$$\begin{aligned}
 \text{Number of molecules of water} &= \text{No. of moles} \times 6.02 \times 10^{23} \\
 &= 0.25 \text{ moles} \times 6.02 \times 10^{23} \text{ molecules per mole} \\
 &= \boxed{1.50 \times 10^{23} \text{ molecules}} \text{ Answer}
 \end{aligned}$$

Example (12):

Mg metal reacts with HCl to give hydrogen gas. What is the minimum volume of HCl solution (27% by weight) required to produce 12.1g of H_2 . The density of HCl solution is 1.14 g/cm^3 .

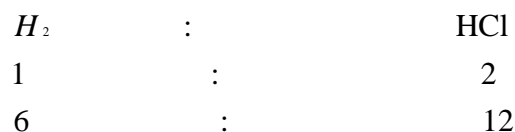


Solution:

$$\begin{aligned}
 \text{Mass of } H_2 \text{ produced} &= 12.1 \text{ g} \\
 \text{Molar mass of } H_2 &= 2.016 \text{ g mol}^{-1}
 \end{aligned}$$

$$\text{Moles of } H_2 = \frac{\text{Mass of } H_2}{\text{Molar mass of } H_2} = \frac{12.1 \text{ g}}{2.016 \text{ g mol}^{-1}} = 6.0 \text{ moles}$$

To calculate the number of moles of HCl, compare the moles of H_2 with those of HCl



So, 12 moles of HCl are being consumed to produce 6 moles of H_2 .

$$\begin{aligned}
 \text{Mass of HCl} &= \text{Moles of HCl} \times \text{Molar mass of HCl} \\
 &= 12 \text{ moles} \times 36.5 \text{ g mol}^{-1} \\
 &= 438 \text{ grams}
 \end{aligned}$$

We know that HCl solution is 27% by weight, it means that 27 g of HCl are present in HCl solution = 100 g

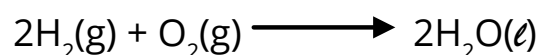
$$\begin{aligned}
 1 \text{ g is present in HCl solution} &= \frac{100}{27} \\
 438 \text{ g are present in HCl solution} &= \frac{100}{27} \times 438 = 1622.2 \text{ g} \\
 \text{Density of HCl solution} &= 1.14 \text{ g/cm}^3 \\
 \text{Volume of HCl} &= \frac{\text{Mass of HCl solution}}{\text{Density of HCl}} \\
 &= \frac{1622.2 \text{ g}}{1.14 \text{ gcm}^{-3}} = \boxed{1423 \text{ cm}^3} \text{ Answer}
 \end{aligned}$$

1.7 LIMITING REACTANT

Having completely understood the theory of stoichiometry of the chemical reactions, we shift towards the real stoichiometric calculations. Real in the sense that we deal with such calculations very commonly in chemistry. Often, in experimental work, one or more reactants is/are deliberately used in excess quantity. The quantity exceeds the amount required by the reaction's stoichiometry. This is done, to ensure that all of the other expensive reactant is completely used up in the chemical reaction. Sometimes, this strategy is employed to make reactions occur faster. For example, we know that a large quantity of oxygen in a chemical reaction makes things burn more rapidly. In this way excess of oxygen is left behind at the end of reaction and the other reactant is consumed earlier. This reactant which is consumed earlier is called a limiting reactant. In this way, the amount of product that forms is limited by the reactant that is completely used. Once this reactant is consumed, the reaction stops and no additional product is formed. **Hence the limiting reactant is a reactant that controls the amount of the product formed in a chemical reaction due to its smaller amount.**

The concept of limiting reactant is analogous to the relationship between the number of "kababs" and the "slices" to prepare "sandwiches". If we have 30 "kababs" and five breads "having 58 slices", then we can only prepare 29 "sandwiches". One "kabab" will be extra (excess reactant) and "slices" will be the limiting reactant. It is a practical problem that we can not purchase exactly sixty "slices" for 30 "kababs" to prepare 30 "sandwiches".

Consider the reaction between hydrogen and oxygen to form water.



When we take 2 moles of hydrogen (4g) and allow it to react with 2 moles of oxygen (64g), then we will get only 2 moles (36 g) of water. Actually, we will get 2 moles (36g) of water because 2 moles (4g) of hydrogen react with 1 mole (32 g) of oxygen according to the balanced equation. Since less hydrogen is present as compared to oxygen, so hydrogen is a limiting reactant. If we would have reacted 4 moles (8g) of hydrogen with 2 moles (64 g) of oxygen, we would have obtained 4 moles (72 g) of water.

Identification of Limiting Reactant

To identify a limiting reactant, the following three steps are performed.

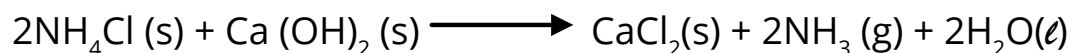
1. Calculate the number of moles from the given amount of reactant.
2. Find out the number of moles of product with the help of a balanced chemical equation.
3. Identify the reactant which produces the least amount of product as limiting reactant.

Following numerical problem will make the idea clear.

Example (13):

NH_3 gas can be prepared by heating together two solids NH_4Cl and $\text{Ca}(\text{OH})_2$. If a mixture containing 100 g of each solid is heated then

- (a) Calculate the number of grams of NH_3 produced.
- (b) Calculate the excess amount of reagent left unreacted.



Solution:

(a) Convert the given amounts of both reactants into their number of moles.

$$\begin{aligned}
 \text{Mass of NH}_4\text{Cl} &= 100\text{g} \\
 \text{Molar mass of NH}_4\text{Cl} &= 53.5\text{g mol}^{-1} \\
 \text{Mass of NH}_4\text{Cl} &= \frac{100\text{g}}{53.5\text{g mol}^{-1}} = 1.87 \\
 \text{Mass of Ca(OH)}_2 &= 100\text{g} \\
 \text{Molar mass of Ca(OH)}_2 &= 74\text{g mol}^{-1} \\
 \text{Moles of Ca(OH)}_2 &= \frac{100\text{g}}{74\text{g mol}^{-1}} = 1.35
 \end{aligned}$$

Compare the number of moles of NH_4Cl with those of NH_3

$$\begin{array}{rcl}
 \text{NH}_4\text{Cl} & : & \text{NH}_3 \\
 2 & : & 2 \\
 1 & : & 1 \\
 1.87 & : & 1.87
 \end{array}$$

Similarly compare the number of moles of Ca(OH)_2 with those of NH_3 .

$$\begin{array}{rcl}
 \text{Ca(OH)}_2 & : & \text{NH}_3 \\
 1 & : & 2 \\
 1.35 & : & 2.70
 \end{array}$$

Since the number of moles of NH_3 produced by 100g or 1.87 moles of NH_4Cl are less, so NH_4Cl is the limiting reactant. The other reactant, Ca(OH)_2 is present in excess. Hence

$$\begin{aligned}
 \text{Mass of NH}_3 \text{ produced} &= 1.87 \text{ moles} \times 17 \text{ g mol}^{-1} \\
 &= \boxed{31.79 \text{ g}} \text{ Answer}
 \end{aligned}$$

(b) Amount of the reagent present in excess

Let us calculate the number of moles of Ca(OH)_2 which will completely react with 1.87 moles of NH_4Cl with the help of equation. For this purpose, compare NH_4Cl and Ca(OH)_2

$$\begin{array}{rcl}
 \text{NH}_4\text{Cl} & : & \text{Ca(OH)}_2 \\
 2 & : & 1 \\
 1 & : & \frac{1}{2} \\
 1.87 & : & 0.935
 \end{array}$$

Hence the number of moles of Ca(OH)_2 which completely react with 1.87 moles of NH_4Cl is 0.935 moles.

No. of moles of Ca(OH)_2 taken = 1.35

No. of moles of Ca(OH)_2 used = 0.935

No. of moles of Ca(OH)_2 left behind = $1.35 - 0.935 = 0.415$

Mass of Ca(OH)_2 left unreacted (excess) = $0.415 \times 74 = \boxed{30.71 \text{ g}}$ Answer

It means that we should have mixed 100 g of NH_4Cl with 69.3 g ($100 - 30.71$) of Ca(OH)_2 to get 1.87 moles of NH_3 .

1.8 YIELD

The amount of the products obtained in a chemical reaction is called the actual yield of that reaction. The amount of the products calculated from the balanced chemical equation represents the theoretical yield. The theoretical yield is the maximum amount of the product that can be produced by a given amount of a reactant, according to balanced chemical equation.

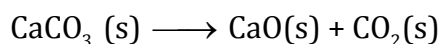
In most chemical reactions the amount of the product obtained is less than the theoretical yield. There are various reasons for that. A practically inexperienced worker has many shortcomings and cannot get the expected yield. The processes like filtration, separation by distillation, separation by a separating funnel, washing, drying and crystallization if not properly carried out, decrease the actual yield. Some of the reactants might take part in a competing side reaction and reduce the amount of the desired product. So in most of the reactions the actual yield is less than the theoretical yield.

A chemist is usually interested in the efficiency of a reaction. The efficiency of a reaction is expressed by comparing the actual and theoretical yields in the form of percentage (%) yield.

$$\% \text{ yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100$$

Example (14):

When lime stone (CaCO_3) is roasted, quicklime (CaO) is produced according to the following equation. The actual yield of CaO is 2.5 kg, when 4.5 kg of lime stone is roasted. What is the percentage yield of this reaction.

**Solution:**

Mass of limestone roasted	= 4.5 kg = 4500 g
Mass of quick lime produced (actual yield)	= 2.5 kg = 2500 g
Molar mass of CaCO_3	= 100 g mol ⁻¹
Molar mass of CaO	= 56 g mol ⁻¹

According to the balanced chemical equation

100 g of CaCO_3 should give CaO	= 56 g
1g of CaCO_3 should give CaO	= 56 / 100
4500 g of CaCO_3 should give CaO	= 56 / 100 x 4500
	= 2520 g
Theoretical yield of CaO	= 2520 g
Actual yield of CaO	= 2500 g

$$\begin{aligned} \% \text{ yield} &= \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100 = \frac{2500\text{g}}{2520\text{g}} \times 100 \\ &= \boxed{99.2 \%} \text{ Answer} \end{aligned}$$

KEY POINTS

1. Atoms are the building blocks of matter. Atoms can combine to form molecules. Covalent compounds mostly exist in the form of molecules. Atoms and molecules can either gain or lose electrons, forming charged particles called ions. Metals tend to lose electrons, becoming positively charged ions. Non-metals tend to gain electrons forming negatively charged ions. When X-rays or α -particles are passed through molecules in a gaseous state, they are converted into molecular ions.
2. The atomic mass of an element is determined with reference to the mass of carbon as a standard element and is expressed in amu. The fractional atomic masses can be calculated from the relative abundance of isotopes. The separation and identification of isotopes can be carried out by mass spectrograph.
3. The composition of a substance is given by its chemical formula. A molecular substance can be represented by its empirical or a molecular formula. The empirical and molecular formula are related through a simple integer.
4. Combustion analysis is one of the techniques to determine the empirical formula and then the molecular formula of a substance by knowing its molar mass.
5. A mole of any substance is the Avogadro's number of atoms or molecules or formula units of that substance.
6. The study of quantitative relationship between the reactants and the products in a balanced chemical equation is known as stoichiometry. The mole concept can be used to calculate the relative quantities of reactants and products in a balanced chemical equation.
7. The concept of molar volume of gases helps to relate solids and liquids with gases in a quantitative manner.
8. A limiting reactant is completely consumed in a reaction and controls the quantity of products formed.
9. The theoretical yield of a reaction is the quantity of the products calculated with the help of a balanced chemical equation. The actual yield of a reaction is always less than the theoretical yield. The efficiency of a chemical reaction can be checked by calculating its percentage yield.

EXERCISE

Q1 Select the most suitable answer from the given ones in each question.

- (i) Isotopes differ in
- (a) properties which depend upon mass
 - (b) arrangement of electrons in orbitals
 - (c) chemical properties
 - (d) the extent to which they may be affected in electromagnetic field.
- (ii) Select the most suitable answer from the given ones in each question.
- (a) Isotopes with even atomic masses are comparatively abundant.
 - (b) Isotopes with odd atomic masses are comparatively abundant.
 - (c) Isotopes with even atomic masses and even atomic numbers are comparatively abundant.
 - (d) Isotopes with even atomic masses and odd atomic numbers are comparatively abundant.
- (iii) Many elements have fractional atomic masses. This is because
- (a) the mass of the atom is itself fractional.
 - (b) atomic masses are average masses of isobars.
 - (c) atomic masses are average masses of isotopes.
 - (d) atomic masses are average masses of isotopes proportional to their relative abundance.
- (iv) The mass of one mole of electrons is
- (a) 1.008 mg
 - (b) 0.55 mg
 - (c) 0.184 mg
 - (d) 1.673 mg
- (v) 27 g of Al will react completely with how much mass of O_2 to produce Al_2O_3 .
- (a) 8 g of oxygen
 - (b) 16 g of oxygen
 - (c) 32 g of oxygen
 - (d) 24 g of oxygen
- (vi) The number of moles of CO_2 which contain 8.0 g of oxygen.
- (a) 0.25
 - (b) 0.50
 - (c) 1.0
 - (d) 1.50
- (vii) The largest number of molecules are present in
- (a) 3.6g of H_2O
 - (b) 4.8g of C_2H_5OH
 - (c) 2.8g of CO
 - (d) 5.4g of N_2O_5
- (viii) One mole of SO_2 contains
- (a) 6.02×10^{23} atoms of oxygen
 - (b) 18.1×10^{23} molecules of SO_2
 - (c) 6.02×10^{23} atoms of sulphur
 - (d) 4 gram atoms of SO_2
- (ix) The volume occupied by 1.4 g of N_2 at S.T.P is
- (a) 2.24 dm³
 - (b) 22.4 dm³
 - (c) 1.12 dm³
 - (d) 112 cm³
- (x) A limiting reactant is the one which
- (a) is taken in lesser quantity in grams as compared to other reactants.
 - (b) is taken in lesser quantity in volume as compared to the other reactants.
 - (c) gives the maximum amount of the product which is required.
 - (d) gives the minimum amount of the product under consideration.

Q 2. Fill in the blanks

- (i) The unit of relative atomic mass is _____.
- (ii) The exact masses of isotopes can be determined by _____ spectrograph.
- (iii) The phenomenon of isotopy was first discovered by _____.
- (iv) Empirical formula can be determined by combustion analysis for those compounds which have _____ and _____ in them.
- (v) A limiting reagent is that which controls the quantities of _____.
- (vi) 1 mole of glucose has _____ atoms of carbon, _____ of oxygen and _____ of hydrogen.
- (vii) 4g of CH_4 at 0°C and 1 atm pressure has _____ molecules of CH_4 .
- (viii) Stoichiometric calculations can be performed only when _____ is obeyed.

Q3. Indicate true or false as the case may be:

- (i) Neon has three isotopes and the fourth one with atomic mass 20.18 amu.
- (ii) Empirical formula gives the information about the total number of atoms present in the molecule.
- (iii) During combustion analysis $\text{Mg}(\text{ClO}_4)_2$ is employed to absorb water vapours.
- (iv) Molecular formula is the integral multiple of empirical formula and the integral multiple can never be unity.
- (v) The number of atoms in 1.79 g of gold and 0.023 g of sodium are equal.
- (vi) The number of electrons in the molecules of CO and N_2 are 14 each, so 1 g of each gas will have same number of electrons.
- (vii) Avogadro's hypothesis is applicable to all types of gases i.e. ideal and non-ideal.
- (viii) Actual yield of a chemical reaction may be greater than the theoretical yield.

Q.4 What are ions? Under what conditions are they produced?

- Q.5 (a) What are isotopes? How do you deduce the fractional atomic masses of elements from the relative isotopic abundance? Give two examples in support of your answer.
- (b) How does a mass spectrograph show the relative abundance of isotopes of an element?
- (c) What is the justification of two strong peaks in the mass spectrum for bromine; while for iodine only one peak at 127 amu is indicated?

Q.6 Silver has atomic number 47 and has 16 known isotopes but two occur naturally i.e. Ag-107 and Ag-109. Given the following mass spectrometric data, calculate the average atomic mass of silver.

Isotopes	Mass (amu)	Percentage abundance
^{107}Ag	106.90509	51.84
^{109}Ag	108.90476	48.16

Q.7 Boron with atomic number 5 has two naturally occurring isotopes. Calculate the percentage abundance of ^{10}B and ^{11}B from the following informations.

Average atomic mass of boron = 10.81 amu

Isotopic mass of ^{10}B = 10.0129 amu

Isotopic mass of ^{11}B = 11.0093 amu (Ans: 20.002%, 79.992)

Q.8 Define the following terms and give three examples of each.

- | | |
|-------------------------------|----------------------|
| 1. Gram atom | 5. Molar volume |
| 2. Gram molecular mass | 6. Avogadro's number |
| 3. Gram formula | 7. Stoichiometry |
| 4. Gram ion | 8. Percentage yield |

Q.9 Justify the following statement!:

- 23 g of sodium and 238 g of uranium have equal number of atoms in them.
- Mg atom is twice heavier than that of carbon atom.
- 180 g of glucose and 342 g of sucrose have the same number of molecules but different number of atoms present in them.
- 4.9 g of H_2SO_4 when completely ionized in water, have equal number of positive and negative charges but the number of positively charged ions are twice the number of negatively charged ions.
- One mg of K_2CrO_4 has thrice the number of ions than the number of formula units when ionized in water.
- Two grams of H_2 , 16 g of CH_4 and 44 g of CO_2 occupy separately the volumes of 22.414 dm^3 , although the sizes and masses of molecules of three gases are very different from each other.

Q.10 Calculate each of the following quantities.

a) Mass in grams of 2.74 moles of KMnO_4 .	• (Ans: 432.92g)
b) Moles of O atoms in 9.00g of $\text{Mg}(\text{NO}_3)_2$.	• (Ans: 0.36 mole)
c) Number of O atoms in 10.037g of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$.	• (Ans: 2.18×10^{23} atoms)
d) Mass in kilograms of 2.6×10^{20} molecules of SO_2 .	• (Ans: 2.70×10^{-5} kg)
e) Moles of Cl atoms in 0.822 g $\text{C}_2\text{H}_4\text{Cl}_2$.	• (Ans: 0.0178 moles)
f) Mass in grams of 5.136 moles of Ag_2CO_3 .	• (Ans: 1416.2 g)
g) Mass in grams of 2.78×10^{21} molecules of CrO_2Cl_2 .	• (Ans: 0.7158 g)
h) Number of moles and formula units in 100g of KClO_3 .	• (Ans: 0.816 moles, 4.91×10^{23} formula units)
i) Number of K^+ ions, ClO_3^- ions, Cl atoms, and O atoms in (h).	• (Ans: $4.91 \times 10^{23} \text{K}^+$, $4.91 \times 10^{23} \text{ClO}_3^-$, $4.91 \times 10^{23} \text{Cl}^-$, 1.47×10^{24} O atoms)

Q.11 Aspartame, the artificial sweetener, has a molecular formula of $\text{C}_{14}\text{H}_{18}\text{N}_2\text{O}_5$.

- a) What is the mass of one mole of aspartame? (Ans: 294 g mol⁻¹)
- b) How many moles are present in 52 g of aspartame? (Ans: 0.177 mole)
- c) What is the mass in grams of 10.122 moles of aspartame? (Ans: 2975.87)
- d) How many hydrogen atoms are present in 2.43 g of aspartame? (Ans: 8.96×10^{22} atoms of H)

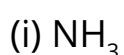
Q.12 A sample of 0.600 moles of a metal M reacts completely with excess of fluorine to form 46.8g of MF_2 .

- a) How many moles of F are present in the sample of MF_2 that forms? (Ans: 1.2 moles)
- b) Which element is represented by the symbol M? (Ans: calcium)

Q.13 In each pair, choose the larger of the indicated quantity, or state if the samples are equal.

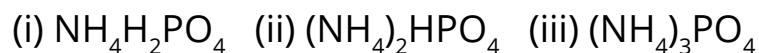
- a) Individual particles: 0.4 mole of oxygen molecules or 0.4 mole of oxygen atoms.
(Ans: both are equal)
- b) Mass: 0.4 mole of ozone molecules or 0.4 mole of oxygen atoms. (Ans: ozone)
- c) Mass: 0.6 mole of C_2H_4 or 0.6 mole of I_2 . (Ans: I_2)
- d) Individual particles: 4.0 g N_2O_4 or 3.3 g SO_2 . (Ans: SO_2)
- e) Total ions: 2.3 moles of NaClO_3 or 2.0 moles of MgCl_2 . (Ans: MgCl_2)
- f) Molecules: 11.0 g H_2O or 11.0 g H_2O_2 . (Ans: H_2O)
- g) Na^+ ion: 0.500 moles of NaBr or 0.0145 kg of NaCl . (Ans: NaBr)
- h) Mass: 6.02×10^{23} atoms of ^{235}U or 6.02×10^{23} atoms of ^{238}U . (Ans: U^{238})

Q.14 a) Calculate the percentage of nitrogen in the four important fertilizers i.e.,



(Ans: 82.35%, 46.67%, 21.21%, 35%)

b) Calculate the percentage of nitrogen and phosphorus in each of the following:



(Ans: (i) N=12.17%, P=26.96% (ii) N=21.21%, P=23.48% (iii) N=28.18%, P=20.81%)

Q.15 Glucose $\text{C}_6\text{H}_{12}\text{O}_6$ is the most important nutrient in the cell for generating chemical potential energy. Calculate the mass % of each element in glucose and determine the number of C, H and O atoms in 10.5 g of the sample.

(Ans: C=40%, H=6.66%, O =53.33%, C=2.107x10²³, H=4.214x10²³, O=2.107x 10²³)

Q.16 Ethylene glycol is used as automobile antifreeze. It has 38.7% carbon, 9.7 % hydrogen and 51.6% oxygen. Its molar mass is 62.1 grams mol⁻¹. Determine its empirical formula.?

(Ans: CH_3O)

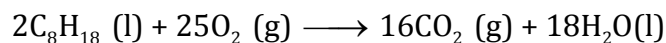
Q.17 Serotonin (Molar mass = 176g mol⁻¹) is a compound that conducts nerve impulses in brain and muscles. It contains 68.2 % C, 6.86 % H, 15.09 % N, and 9.08 % O. What is its molecular formula.

(Ans: $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}$)

Q.18 An unknown metal M reacts with S to form a compound with a formula M_2S_3 . If 3.12 g of M reacts with exactly 2.88 g of sulphur, what are the names of metal M and the compound M_2S_3 ?

(Ans: Cr; Cr_2S_3)

Q.19 The octane present in gasoline burns according to the following equation.



a) How many moles of O_2 are needed to react fully with 4 moles of octane?

(Ans: 50 moles)

b) How many moles of CO_2 can be produced from one mole of octane?

(Ans: 8 moles)

c) How many moles of water are produced by the combustion of 6 moles of octane?

(Ans: 54 moles)

d) If this reaction is to be used to synthesize 8 moles of CO_2 how many grams of oxygen are needed? How many grams of octane will be used?

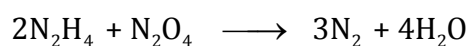
(Ans: 400 g; 114 g)

Q.20 Calculate the number of grams of Al_2S_3 which can be prepared by the reaction of 20 g of Al and 30 g of sulphur. How much the non-limiting reactant is in excess?

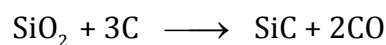
(Ans: 46.87g; 3.125g)

Q.21 A mixture of two liquids, hydrazine N_2H_4 and N_2O_4 are used in rockets. They produce N_2 and water vapours. How many grams of N_2 gas will be formed by reacting 100 g of N_2H_4 and 200g of N_2O_4 .

(Ans: 131.04g)



Q.22 Silicon carbide (SiC) is an important ceramic material. It is produced by allowing sand (SiO_2) to react with carbon at high temperature.



When 100 kg sand is reacted with excess of carbon, 51.4 kg of SiC is produced. What is the percentage yield of SiC? (Ans: 77%)

- Q.23 a. What is stoichiometry? Give its assumptions? Mention two important laws, which help to perform the stoichiometric calculations?
b. What is a limiting reactant? How does it control the quantity of the product formed? Explain with three examples?
- Q.24 a. Define yield. How do we calculate the percentage yield of a chemical reaction?
b. What are the factors which are mostly responsible for the low yield of the products in chemical reactions?
- Q.25 Explain the following with reasons.
- Law of conservation of mass has to be obeyed during stoichiometric calculations.
 - Many chemical reactions taking place in our surrounding involve the limiting reactants.
 - No individual neon atom in the sample of the element has a mass of 20.18 amu.
 - One mole of H_2SO_4 should completely react with two moles of NaOH. How does Avogadro's number help to explain it.
 - One mole of H_2O has two moles of bonds, three moles of atoms, ten moles of electrons and twenty eight moles of the total fundamental particles present in it.
 - N_2 and CO have the same number of electrons, protons and neutrons.