Mole Concept and Stoichiometry

Concept

Mole Concept

Introduction

This is our common experience that when we go to market to buy something, a few things we always get in definite numbers. For example, eggs we get in a number of 12 which is called a **dozen ,** playing cards we get in a number of 52 which is called **a pack**, papers we get in a number of 480 sheets which is called a **ream.** Dozen, pack and ream are units to describe those items. Following chart shows certain items which we get in definite numbers and the units in which these items are described.

Substance	Unit	Number
Drawing pins	Gross	144
Football boots	Pair	2
Eggs	Dozen	12
Playing cards	Pack	52
Paper	Ream	480 sheets
Carbon	Mole	6.02×10^{23} particles

What is a mole ?

In Latin, mole means 'massive heap' of material. In chemistry, it is a unit which is used to describe an amount of atoms, ions and molecules. It enables chemists to count these particles by weighing.

According to 14th conference of National Institutes of Standards and Technology (NIST) held in 1971, the definition of mole is given as follows.

Mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon – 12. Its symbol is mol.

When the mole is used, the elementary entities must be specified and they may be atoms, molecules, ions, electrons, other particles or specified group of such particles.

Visualizing a mole as a pile of particles, however, is just one way to understand this concept. A sample of a substance has mass, volume (generally used with gases) and number of particles that is proportional to the chemical amount (measured in moles) of the sample. For example, one mole of oxygen (O_2) occupies a volume of 22.4 liters at

standard temperature and pressure (STP = O^0 C and 1 atm), has a mass of 31.998 grams and contains about 6.022 x 10^{23} molecules of oxygen. Measuring one of these quantities allows the calculation of the others and this is frequently done in stoichiometry.

One interpretation : A specific number of particles

When a quantity of particles is to be described, mole is a grouping unit analogous to groupings such as pair, dozen or gross, in that all of these words represent specific numbers of objects. The main difference between the mole and the other grouping units is the magnitude of the number represented and how that number is obtained. One mole is an amount of substance containing Avogadro's number of particles. Avogadro's number is equal to 6.02214199 x 10^{23} .

Unlike pair, dozen and gross, the exact number of particles in a mole can not be counted. There are several reasons for this. First, the particles are too small and can not be seen even with a microscope. Second, as naturally occurring carbon contains approximately 98.90 % carbon – 12, the sample would need to be purified to remove every atom of carbon – 13 and carbon – 14. Third, as the number of particles in a mole is tied to the mass of exactly 12 grams of carbon – 12, a balance would need to be constructed that could determine if the sample was one atom over or under exactly 12 grams. If the first two requirements were met, it would take one million machines counting one million atoms each second more than 19,000 years to complete the task. So, practically it can be treated as impossible though is theoretically possible.

Obviously, if the number of particles in a mole can not be counted, the value must be measured indirectly and with every measurement there is some degree of uncertainty. Therefore, the number of particles in a mole, Avogadro's constant (N_A) can only be approximately found through experimentation and thus its reported values will vary slightly (at the tenth decimal place) based on the method used for measurement. . Most methods agree to four significant figures , so N_A is generally said to equal 6.022 x 10^{23} particles per mole and this value is usually sufficient for solving common problems. Another key point is that the formal definition of a mole does not include a value for Avogadro's constant and this is probably due to the inherent uncertainty in its measurement. As for the difference between Avogadro's constant and Avogadro's number, they are numerically equivalent but the former has the unit of mol^{-1} whereas the latter is a pure number with no unit.

Avogadro's constant is related to the number of atoms or molecules present in the volume occupied by one mole of a gas at S.T.P. conditions or it is the number of atoms or molecules present in one mole of a substance. Avogadro's number is a pure number just as dozen or gross and it is dimensionless. It equals the number of particles (electrons, atoms, ions, molecules etc.) of anything which is numerically equivalent to the number of atoms present in 0.012 kg of carbon – 12.

Activity 1 - In a boys hostel, 1206 eggs were brought for the breakfast of students. What is the number of moles of eggs brought ?

A second interpretation : A specific mass

Atoms and molecules are incredibly small and even a tiny chemical sample contains an unimaginable number of them. Therefore, counting the number of atoms or molecules in a sample is impossible. The multiple interpretations of the mole allow us to bridge the gap between the submicroscopic world of atoms and molecules and the macroscopic world that we can observe.

To determine the chemical amount of a sample, we use the substance's molar mass, the mass per mole of particles. We will use carbon – 12 as an example because it is the standard for the formal definition of the mole. According to definition, one mole of carbon – 12 is 12 g/mol. However the molar mass for the element carbon is 12.011 g/mol. Why are they different ? To answer that question, few terms need to be clarified.

In the periodic table, we observe that most of the atomic weights are not integers. The atomic weight is a weighed average of the atomic masses of the natural isotopes of the element. For example, bromine has two natural isotopes with atomic masses of 79 u and 81 u. The unit u represents the atomic mass unit and is used in place of grams because the value would be inconveniently small. These two isotopes of bromine are present in nature in almost equal amounts, so the atomic weight of the element bromine is 79.904 (i.e. nearly 80, the arithmetic mean of 79 and 81). A similar situation exists for chlorine but chlorine – 35 is almost three times as abundant as chlorine – 37, so the atomic weight of chlorine is 35.4527. Technically, atomic weights are ratios of the average atomic mass to the unit u and that is why they do not have units. Sometimes, atomic weights are given the unit u but this is not quite correct according to the International Union of Pure and Applied Chemistry (IUPAC).

To find the molar mass of an element or compound, determine the atomic, molecular or formula weight and express that value as g/mol. For bromine and chlorine, the molar masses are 79.904 g/mol and 35.4527 g/mol respectively. Sodium chloride (NaCl) has a formula weight of 58.443 (atomic weight of Na + atomic weight of Cl) and a molar mass of 58.443 g / mol. Formaldehyde (CH_2O) has a molecular weight 30.03 (atomic weight of C + 2 [atomic weight of H] + atomic weight of O) and a molar mass of 30.03 g/mol.

The concept of molar mass enables chemist to measure the number of submicroscopic particles in a sample without counting them directly simply by determining the chemical amount (in grams)of a sample. To find the chemical amount of a sample, chemists measure its mass and divide by its molar mass. Multiplying the chemical amount (in moles) by Avogadro's constant (N_A) yields the number of particles present in the sample.

Occasionally, one encounters the terminology - gram-atomic mass (GAM) gram-formula mass (GFM) and gram- molecular mass (GMM). These terms are functionally the same as molar mass . For example, the GAM of an element is the mass in grams of a sample containing N_A atoms and is equal to the element's atomic weight expressed in grams. For example, the GAM of oxygen is 16 g which contains 6.023×10^{23} atoms of oxygen. GFM and GMM are defined similarly. Other terms you may come across are formula mass and molecular mass. Interpret these as formula weight and molecular weight respectively but with the units of u.

Activity 2 - In a photosynthesis reaction, a plant releases 1.0×10^{12} molecules of O_2. What is the mass of oxygen released ?

Avogadro's Hypothesis

Some people think that Avogadro (1776 – 1856) determined the number of particles in a mole and that is why the quantity is known as Avogadro's number. In reality, Avogadro built a theoretical foundation for determining accurate atomic and molecular masses. The concept of mole did not even exist in Avogadro's time.

Much of Avogadro's work was based on that of Gay-Lussac (1778 – 1850) . Gay – Lussac developed the law of combining volumes which states that ' In any chemical reaction involving gaseous substance, the volumes of various gases reacting or produced are in the ratios of small whole numbers.'. Avogadro reinterpreted Gay-Lussac's findings and proposed in 1811 that (i) some molecules were diatomic and (ii) equal volumes of all gases at the same temperature and pressure contain the same number of molecules. The second proposal is what we refer to as Avogadro's hypothesis.

The hypothesis provided a simple method of determining relative molecular weights because equal volumes of two different gases at the same temperature and pressure contained the same number of particles, so the ratio of the masses of the gas samples must also be that of their particle masses. Unfortunately, Avogadro's hypothesis was largely ignored until Cannizzaro (1826- 1910) advocated using it to calculate relative atomic masses or atomic weights. Soon after the first International Chemical Congress at Karlsrule in 1860, Cannizzaro's proposal was accepted and a scale of atomic weights was established.

To understand how Avogadro's hypothesis can be used to determine relative atomic and molecular masses, imagine two identical boxes with oranges in one and grapes in the other. The exact number of fruits in each box is not known. But you believe that there are equal number of fruits in each box (Avogadro's hypothesis). After subtracting the masses of the boxes, you have the masses of each fruit sample and can determine the mass ratio between the oranges and the grapes. By assuming that there are equal numbers of fruits in each box, you then know the average mass ratio between a grape and an orange, so in effect you have calculated their relative masses (atomic masses). If you chose either the grape or the orange as a standard, you could eventually determine a scale of relative masses for all fruits.

A third interpretation : A specific volume

By extending Avogadro's hypothesis, there is a specific volume of gas that contains N_A gas particles for a given temperature and pressure and that volume should be the same for all gases. For an ideal gas, the volume of one mole at STP (0^0C and 1 atm) is 22.4 liters and several real gases (like hydrogen, oxygen and nitrogen) come very close to this value.

Activity 3 – In a combustion reaction, 132 grams of CO_2 was produced. What is the volume occupied by this CO_2 at STP ?

The size of Avogadro's number

To give some idea of the enormous magnitude of Avogadro's number, let us take some examples. Avogadro's number of water drops (twenty drops per ml) would fill a rectangular column of water 9.2 km (5.7 miles) by 9.2 km (5.7 miles)at the base and reaching to the moon at perigee (closest distance to earth). Avogadro's number of water drops would cover all of the land in the United States to a depth of approximately 3.3 km (about 2 miles). Avogadro's number of rupees placed in a rectangular stack roughly 6 meters by 6 meters at the base would stretch for about 9.4×10^{12} km and extend outside of our solar system. It would take light nearly an year to travel from one end of the stack to the other.

Check your understanding :

1) Calculate the number of molecules in 1 kg of sodium hydroxide.
(Answer – 1.506×10^{25})

2) Calculate the molecular weight of a gas which at STP weigh 0.48 g and occupies a volume of 100 ml ? (Answer – 107.5)

3) Calculate the number of moles in 3.011×10^{23} atoms of calcium .
(Answer – 0.5 mole)

4) Which represents greatest mass among 100 gm of calcium, 3 g-atoms of calcium , 1 mole of calcium oxide, 10^{25} molecules of oxygen?
(Answer - 10^{25} molecules of oxygen)

Concept

Applications of Avogadro's law

Avogadro's law has been used at number of places. Some of its applications are described below.

1) **To determine atomicity of gases**

The number of atoms present in one molecule of an element is called its atomicity. Consider the following reaction:

Hydrogen + Chlorine → Hydrogen chloride

1 volume	1 volume	2 volumes	(According to Gay-Lussac's law)
n molecules	n molecules	2n molecules	(According to Avogadro's law)

1 atom	1 atom	2 compound - atoms (molecules)
½ atom	½ atom	1 molecule

1 molecule of hydrogen chloride = ½ molecule of hydrogen + ½ molecule of chlorine
But ½ molecule of hydrogen = 1 atoms of hydrogen . So
1 molecule of hydrogen = 2 atoms of hydrogen

Hence atomicity of hydrogen molecule is 2.

Activity 1 - One volume of nitrogen combines with three volumes of hydrogen to form two volumes of ammonia gas. Determine the atomicity of nitrogen gas.

2) **Explanation of Gay – Lussac's law of combining volumes**

Gay – Lussac suggested that one volume of hydrogen and one volume of chlorine react to produce two volumes of hydrogen chloride gas.
According to Avogadro's law if,

1 volume of hydrogen contains	n molecules of the gas, then
1 volume of chlorine also contains	n molecules of the gas
2 volumes of hydrogen chloride contain	2n molecules of the gas

Hydrogen + Chlorine → Hydrogen chloride

1 volume	1 volume	2 volumes	(According to Gay-Lussac's law)
n molecules	n molecules	2n molecules	(According to Avogadro's law)

But hydrogen and chlorine are diatomic.

2 atoms	2 atoms	2 molecules
1 atom	1 atom	1 molecule

It is seen that 1 molecule of hydrogen chloride is formed when 1 atom of hydrogen combines with 1 atom of chlorine.
Thus, Avogadro's law explains Gay – Lussac's law of combining volumes.

3) **Modification of Dalton's atomic theory**

Avogadro suggested the presence of two particles – an atom and a molecule.
An atom is the smallest particle of an element that can take part in a chemical reaction. It does not have independent existence and it can not be split into similar particles.
A molecule is the smallest particle of matter that exists in free state. It is made up of two or more atoms of the same or different elements. A molecule can be divided to give the respective atoms.

Let us take the example of reaction between hydrogen and chlorine.

Hydrogen	Chlorine →	Hydrogen chloride
1 volume	1 volume	2 volumes
n molecules	n molecules	2n molecules (According to Avogadro's hypothesis)
1 molecule	1 molecule	2 molecules
½ molecule	½ molecule	1 molecule

This shows that 1 molecule of hydrogen chloride is formed from ½ molecule of hydrogen and ½ molecule of chlorine. Since molecules can be divided, Avogadro's hypothesis is true.

4) **To derive the relation between molecular weight and vapour density**

According to Avogadro's law,

$$\text{Vapour density at STP} = \frac{\text{Mass of n molecules of a gas or vapour}}{\text{Mass of n molecules of hydrogen}}$$

$$\text{Vapour density} = \frac{\text{Mass of 1 molecule of a gas or vapour}}{\text{Mass of 1 molecule of hydrogen}}$$

$$\text{Vapour density} = \frac{\text{Mass of 1 molecule of a gas or vapour}}{\text{Mass of 2 atoms of hydrogen}}$$

$$\text{Vapour density} = \frac{\text{Mass of 1 molecule of a gas or vapour}}{2 \times (\text{Mass of 1 atoms of hydrogen})}$$

$$\text{Vapour density} = \frac{1}{2} \times \frac{\text{Mass of 1 molecule of a gas or vapour}}{\text{Mass of 1 atom of hydrogen}}$$

$$\text{Vapour density (VD)} = \frac{1}{2} \times \text{Molecular weight}$$

2 x Vapour density (2 V.D) = Molecular weight

Activity 2 - Find out the molecular weight of NO_2 gas and determine its vapour density.

5) **To derive the relation between gram molecular weight (GMW) and gram molecular volume (GMV)**

Density of any gas = Weight of 1 liter of that gas at STP

Let us determine the molar volume of hydrogen (any gas for that matter)

Density of hydrogen = 0.09 g/liter

Molecular weight of hydrogen = 2.016

$$\text{Molar volume} = \frac{\text{Molecular weight in grams}}{\text{Density of hydrogen}} = \frac{2.016}{0.09} = 22.4 \text{ liters}$$

Thus gram molecular masses (one gram mole) of all gases at STP occupy a volume of 22.4 liters .

Activity 3 - Derive the relation between gram molecular volume and vapour density of a volatile compound.

6) **To determine the formula of a gaseous molecule**

Let us take an example of ammonia gas. Experimentally it is proved that two volumes of ammonia on decomposition give one volume of nitrogen and three volumes of hydrogen.

Ammonia →	Nitrogen +	Hydrogen	
2 volumes	1 volume	3 volumes	(According to Gay-Lussac's law)
2 molecules	1 molecule	3 molecules	(According to Avogadro's law)
2 molecules	2 atoms	6 atoms	

(Nitrrogen and hydrogen are diatomic)

1 molecule	1 atom	3 atoms

1 molecule of ammonia = 1 atom of nitrogen + 3 atoms of hydrogen

Hence, molecular formula of ammonia is NH_3.

Activity 4 - Two volumes of nitrogen dioxide, on decomposition, give two volumes of nitric oxide and one volume of oxygen. Prove that molecular formula of nitrogen dioxide is NO_2.

Check your understanding :

1) 500 ml of nitric oxide react with 300 ml of oxygen to form nitrogen dioxide. What is the composition of the resulting mixture ?

(Answer – 500 ml NO_2 + 50 ml O_2)

2) 6 grams of a gas occupies a volume of 700 ml at 70^0C and 70 cm pressure. If 1 liter of hydrogen weighs 0.9 gram at STP, what is the vapour density of the gas ?

(Answer – 13)

3) The molecular weight of a gas is 44. What is the weight of the gas which occupies a volume of 20 liters at 27^0C and 70 cm pressure ?

(Answer - 32.91 gram)

Concept

Stoichiometry

Introduction

Stoichiometry is simply the mathematics behind chemistry. Given enough information, one can use stoichiometry to calculate masses, moles and percents within a chemical equation. It is a mathematical method to calculate quantitative information from chemical formulae or equation of chemical reaction .

Every chemical reaction has its characteristic proportions. Chemical formulae, equations, atomic weights and molecular weights are used to find out these proportions. Determination of what and how much is used and produced in chemical processes is the major concern of stoichiometry.
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What is stoichiometry ?

Stoichiometry is a branch of chemistry that deals with the quantitative relationships that exist among the reactants and products in chemical reactions.

In a balanced chemical reaction, the relations among quantities of reactants and products typically form a proportion of whole numbers. For example, in a reaction that forms ammonia (NH_3), exactly one molecule of nitrogen (N_2) reacts with three molecules of hydrogen (H_2) to produce two molecules of NH_3:

$$N_2 + 3H_2 \rightarrow 2NH_3$$

Stoichiometry can be used to derive various kinds of information from the balanced chemical equation. Depending upon its use, it can be broadly classifies as reaction stoichiometry, composition stoichiometry, gas stoichiometry etc.

1) Reaction stoichiometry describes the quantitative relationships among substances as they participate in chemical reactions. In the example above, reaction stoichiometry describes the 1:3:2 proportion s of molecules of nitrogen, hydrogen, and ammonia.

2) Composition stoichiometry describes the quantitative (mass) relationships among elements in compounds. For example, composition stoichiometry describes the nitrogen to hydrogen (mass) relationship in the compound ammonia i.e. 28 grams of nitrogen react with 6 grams of hydrogen to form 34 grams of ammonia.

Stoichiometry can be used to calculate quantities such as the amount of products that can be produced with given reactants and percent yield (the percentage of the given reactant that is made into the product).

A **stoichiometric amount** or **stoichiometric ratio** of a reagent is the amount or ratio where, it is assumed that the reaction proceeds to completion and :

1. all reagent is consumed,
2. there is no shortfall of reagent, and
3. no residues remain.

3) Gas stoichiometry deals with reactions involving gases, where the gases are at a known temperature, pressure, and volume and can be assumed to be ideal gases. For gases, the volume ratio is ideally the same by the ideal gas law, but the mass ratio of a single reaction has to be calculated from the molecular masses of the reactants and products. In practice, due to the existence of isotopes, molar masses are used instead when calculating the mass ratio.

Stoichiometry is based on the law of conservation of mass. The mass of the reactants equals the mass of the products.

Illustrations

1) **Reaction stoichiometry -** How many moles of magnesium will react with one mole of oxygen ?

A balanced chemical equation for the reaction between magnesium and oxygen can be written as follows.

$$2\ Mg + O_2 \rightarrow 2\ MgO$$

The reaction stoichiometry shows that Mg, O_2 and MgO take part in the reaction in the proportion 2:1:2. So 2 moles of Mg will react with one mole of oxygen.

Activity 1 – Describe the reaction stoichiometry in the following reaction.

$$4\ NH_3\ (g) + 5\ O_2\ (g) \rightarrow 4\ NO\ (g) + 6\ H_2O\ (l)$$

2) Composition stoichiometry - How many grams of oxygen do you need to burn 1.00 gram of Mg? (Note: The balanced equation for this reaction was obtained in the previous question.)

The balanced equation shows that 24 grams (2 moles) of Mg react with 32 grams (1 mole) of oxygen to produce 56 grams (2 moles) of MgO. So 1.33 gram of O_2 will be needed to burn 1 gram of Mg metal.

Activity 2 - Describe the composition stoichiometry in the following reaction.

$$(NH_4)_2Cr_2O_7\ (s) \rightarrow\ Cr_2O_3\ (s)\ +\ N_2\ (g)\ +\ 4\ H_2O\ (g)$$

3) **Gas Stoichiometry** – Calculate the volume of gaseous NO_2 produced at STP from the combustion of 100 grams of NH_3 by the reaction

$$4NH_3\ (g) + 7O_2\ (g) \rightarrow 4NO_2\ (g) + 6H_2O\ (g\ )$$

First we find out the moles of NH_3 . Moles of NH_3 = 100 / 17 = 5.88 moles
There is a 1:1 molar ratio of NH_3 to NO_2 in the above balanced combustion reaction, so 5.88 mol of NO_2 will be formed. We will employ the ideal gas law to solve for the volume at 0 °C (273 K) and 1 atmosphere using the gas law constant of
R = 0.082 L · atm · K^{-1} · mol^{-1} :

PV = n R T or V = n R T / P . Then, V = 5.88 x 0.082 x 273 = 131.6 liters

Activity 3 - Describe the gas stoichiometry in the following reaction.

$$C_3H_8\ (g)\ +\ 5\ O_2\ (g)\ \rightarrow\ 3\ CO_2\ (g)\ +\ 4\ H_2O\ (g)$$

Limiting reagents

Sometimes when reactions occur between two or more substances, one reactant runs out before the other. That is called the "limiting reagent". Often, it is necessary to identify the limiting reagent in a problem.

Illustration:

A chemist only has 6. 50 grams of C_2H_2 and an unlimited supply of oxygen and he desires to produce as much CO_2 as possible. If he uses the equation below, how much oxygen should he add to the reaction?

$$2C_2H_2\ (g\ ) + 5O_2(g) \text{ ---> } 4CO_2(g) + 2\ H_2O(l)$$

Here acetylene, C_2H_2 is the limiting reagent. To solve this problem, it is necessary to determine how much oxygen should be added if all of the reactants were used up (this is the way to produce the maximum amount of CO_2).

First, we calculate the number of moles in 6.50 g of C_2H_2. We know that molecular weight of CO_2 is 26. Therefore 1 mole of C_2H_2 weighs 26 g .Then 6.5 gram of C_2H_2 is equivalent to 6.5 / 26 = 0.25 moles

Then, because there are five (5) molecules of oxygen to every two (2) molecules of C_2H_2, we need to multiply the result by 5/2 to get the total molecules of oxygen. Then we convert to grams to find the amount of oxygen that needs to be added:

0.25 x 5/2 = 0.625 moles of O_2. Since 1 mole of O_2 weighs 32 grams, 0.625 moles of O_2 will weigh 0.625 x 32 = 20 grams

Activity 4 – :If 20.0 g of iron (III) oxide (Fe_2O_3) are reacted with 8.00 g aluminium (Al) in the thermite reaction, which reactant is limiting?

$$Fe_2O_3\ (s) + 2\ Al\ (s) \rightarrow Al_2O_3\ (s) + 2\ Fe\ (l)$$

Check your understanding :

1) A reaction takes place as $Na_3PO_4 + Al(NO_3)_3 \rightarrow AlPO_4 + 3\ NaNO_3$
How many moles of sodium nitrate are produced when two moles of sodium phosphate react with two moles of aluminium nitrate ?

(Answer – 6 moles)

2) What weight of sulphuric acid will be required to dissolve 6 grams of magnesium carbonate according to the equation –

$$MgCO_3 + H_2SO_4 \rightarrow MgSO_4 + H_2O + CO_2\ ?$$

(Answer – 7 grams)

3) Potassium chlorate decomposes as follows.

$$2\ KClO_3 \rightarrow 2\ KCl + 3\ O_2$$

4) If 4.9 grams of $KClO_3$ is decomposed, what volume of O_2 is produced at STP ?

(Answer – 1.344 liters)

Concept

Percentage composition of a compound by mass

Percentage composition of a compound by mass can be defined as follows.

Percentage composition by mass is the mass of solute (or one component) divided by the mass of solute + solvent (mass of all the components) multiplied by 100.

Or

The percentage composition of a compound is a relative measure of the mass of each different element present in the compound.

How to calculate the percentage composition of a compound ?

(i) Calculate the molecular mass, (molecular weight, formula weight or formula mass) MM of the compound.
(ii) Calculate the total mass of each element present in the formula of the compound
(iii) % composition = (total mass of element present / molecular mass) x 100

Illustration

1) Calculate the percent by weight of each element present in sodium sulfate (Na_2SO_4).

Calculate the molecular mass MM of the compound Na_2SO_4.

MM = (2 x 23) + (1 x 32) + (4 x 16) = 142

Total mass of Na present = 2 x 23 = 46
Total mass of S present = 1 x 32 = 32
Total mass of O present = 4 x 16 = 64

% of Na = (46 / 142) x 100 = 32.4 %
% of S = (32 / 142) x 100 = 22.53 %
% of O = (64 / 142) x 100 = 45.07 %
Total percentage = 32.40 + 22.53 + 45.07 = 100

2) Calculate the percent by weight of each element in sodium chloride (NaCl)

Calculate the molecular mass MM of the compound Na Cl

MM = (1 x 23) + (1 x 35.5) = 58.5 .
Total mass of Na present = 1 x 23 = 23
Total mass of Cl present = 1 x 35.5 = 35.5
% of Na = 23 / 58.5 = 39.35 ; % of Cl = 35.5 / 58.5 = 60.65
Total percentage = 39.35 + 60.65 = 100

Activity 1 – Calculate the percent by weight of each element present in calcium phosphate $Ca_3(PO_4)_2$ .Calculate the molecular mass MM of the compound $Ca_3(PO_4)_2$.

Activity 2 – A compound with molecular mass 74 contains elements Ca, O and H. If the % of Ca is 54.09 and that of H is 2.73, find the atomic mass of Ca in the compound.

Check your understanding :

1) Ammonium dichromate $(NH_4)_2Cr_2O_7$ has a molecular mass 252. What is the % of N, H, Cr and O in the compound
(Answer – N = 11.11 %, H = 3.18 %, Cr = 41.27 % , O = 44.44 %)

2) What is the atomic mass of potassium, if the % of nitrogen is 13.9 and that of oxygen is 47.5 in a compound containing K,N and O with molecular mass 101 ?
(Answer – 39)

3) A compound contains the elements Mg, N and O. The percentage of these elements in a compound is 16.2, 18.9 and 64 respectively. What is the molecular weight of this compound ?
(Answer – 148)

Concept

Empirical and Molecular Formula

Introduction

In chemistry, generally we come across three types of formulae of compounds –viz. Empirical formula, Molecular formula and Structural formula.

Empirical formula of a compound shows the ratio of elements present in that compound.

Molecular formula of a compound shows how many atoms of each element are present in a molecule of that compound.

Structural formula of a compound shows the covalent bonds (single, double or triple) between every two atoms and placement of the atoms in the molecule of that compound.

Empirical and Molecular formula

Let us explain empirical and molecular formula in some more details.

Empirical formula represents the simplest whole number ratio of atoms of each element present in a compound. The empirical formula is the molecular formula reduced to its lowest common denominator. The empirical formula makes no reference to isomerism, structure or absolute number of atoms. It does not indicate the actual number of atoms of the elements present in the molecule.

For example, formaldehyde, acetic acid and glucose have the same empirical formula, CH_2O. The elements C, H and O are present in the proportion 1:2:1 in all these compounds. Empirical formula represents the simplest whole number ratio of atoms of each element present in a compound . However, the molecular formulae of formaldehyde, acetic acid and glucose are HCHO, CH_3COOH and $C_6H_{12}O_6$ respectively. Empirical formula and molecular formula are same for formaldehyde. But they are different for acetic acid and glucose. Acetic acid has double the number of atoms and glucose has six times the number of atoms of formaldehyde.

Molecular formula is a group of elemental symbols and possibly subscript numbers which represent the composition of a molecule. Molecular formula shows the exact number of atoms of each element in the molecule or how many atoms of each element are present in the molecule of a compound. In the above examples, all the compounds have the same proportion of C, H and O. But the actual number of atoms of each element are different in formaldehyde, acetic acid and glucose.

Another example is that ethylene (C_2H_4), propene (C_3H_6) and butane (C_4H_8) all have the same empirical formula CH_2 but their molecular formulae are different. They have the same proportion of C to H as 1:2 but actual number of C and H atoms are 1.5 times in propene and 2 times in butene as compared to those in ethylene.

Activity 1 - Write the molecular formula of two cycloalkanes which have the empirical formula CH_2.

Activity 2 – Two organic compounds have the same empirical formula and molecular formula C_2H_6O but different structural formula . Suggest the names of these compounds.

The relation between empirical formula and molecular formula can be given as follows.

Molecular formula = Integer x Empirical formula

It follows then that :

Molecular formula weight = Integer x Empirical formula weight

Check your understanding :

1) Find the empirical formula of a compound of carbon and hydrogen which contains 80 % carbon . (Answer – CH_3)

2) A compound has an empirical formula CH_2O and a vapour density 30. What is its molecular formula ? (Answer – $C_2H_4O_2$)

3) An organic compound contains the elements C, H and Br. Their % in the compound is as follows. C = 12.76 % , H = 2.13 % and Br = 85.11 % The vapour density of the compound is 94. What is the molecular formula of the compound ?
(Answer – $C_2H_4Br_2$)

Concept

How to calculate Empirical Formula from Percentage Composition

Introduction

To calculate empirical formula from percentage composition, we follow the steps :

1) Assume 100g of sample
2) Convert all percentages to a mass in grams, eg, 21% = 21g, 9% = 9g
3) Find the relative atomic mass (r.a.m) of each element present using the Periodic Table
4) Calculate the moles of each element present: n = mass ÷ r.a.m
5) Divide the moles of each element by the smallest of these to get a mole ratio
6) If the numbers in the mole ratio are all whole numbers (integers) convert this to an empirical formula
7) If the numbers in the mole ratio are NOT whole numbers, you will need to further manipulate these until the mole ratio is a ratio of whole numbers (integers).

Recognizing the decimal equivalent of common fractions is very helpful.

Common Decimal	Equivalent Fraction	Mole Ratio Example
0.125	1/8	1 : 1.125 converts to 1 : 9/8 multiply throughout by 8 to give 8 : 9
0.25	1/4	1 : 0.25 converts to 1 : 1/4 multiply throughout by 4 to give 4 : 1
0.33	1/3	1 : 1.33 converts to 1 : 4/3 multiple throughout by 3 to give 3 : 4
0.375	3/8	1 : 1.375 converts to 1 : 11/8 multiply throughout by 8 to give 8 : 11
0.5	1/2	2 : 1.5 converts to 2 : 3/2 multiply throughout by 2 to give 4 : 3
0.625	5/8	1 : 1.625 converts to 1 : 13/8 multiply throughout by 8 to give 8 : 13
0.66	2/3	2 : 1.66 converts to 2 : 5/3 multiply throughout by 3 to give 6 : 5
0.875	7/8	1 : 0.875 converts to 1 : 7/8 multiply throughout by 8 to give 8 : 7

Illustration

1) A compound is found to contain 47.25% copper and 52.75% chlorine. Find the empirical formula for this compound.

Element	Cu	Cl
mass in grams	47.25	52.75
r.a.m	63.6	35.5
moles = mass ÷ r.a.m	47.25 ÷ 63.6 = 0.74	52.75 ÷ 35.5 = 1.49
divide throughout by lowest number	0.74 ÷ 0.74 = 1	1.49 ÷ 0.74 = 2.01 = 2

Empirical formula for this compound is $CuCl_2$

2) A compound with a molecular mass of 34 g/mol is known to contain 5.88 percent hydrogen and 94.12 percent oxygen. Find the molecular formula for this compound.

First find the empirical formula for this compound.

Element	H	O
mass in grams	5.88	94.12
r.a.m	1.0	16.0
moles = mass ÷ r.a.m	5.88 ÷ 1.0 = 5.88	94.12 ÷ 16.0 = 5.88
divide throughout by the smallest number	5.88 ÷ 5.88 = 1	5.88 ÷ 5.88 = 1

Empirical formula is HO

Calculate the empirical formula mass: 1.0 + 16.0 = 17.0 g/mol

Molecular formula weight = Integer x Empirical formula weight

34 = n x 17 So, n = 2

Molecular Formula is 2 x (HO) which is H_2O_2

3) A substance on analysis gave Na = 43.4 %, C = 11.3 % and O = 45.3 % . Find out its empirical and molecular formula.

Element	Na	C	O
%	43.4	11.3	45.3
Atomic mass	23	12	16
Mole = mass / r.a.m.	43.4 / 23 = 1.88	11.3 / 12 = 0.94	45.3 / 16 = 2.83
Simplest ratio	1.88 / 0.94 = 2	0.94 / 0.94 =1	2.83 / 0.94 = 3

Empirical formula is Na_2CO_3. No information is given about the molecular formula weight. A compound with molecular formula Na_2CO_3 does exist. So molecular formula and empirical formula of this compound is same i.e. Na_2CO_3.

Activity 1 - A compound has three elements C, H and O. Their mole % in the compound is 3.331, 6.667 and 3.331 respectively. The molecular mass of the compound is 180. What is the molecular formula of the compound ?

Activity 2 - Given that the empirical formula of a compound is CH and the molar mass is 104 g/mol, calculate the molecular formula.

Check your understanding :

1) A compound contains 68.85 % carbon, 4.92 % hydrogen and 26.23 % oxygen. Find the empirical formula of the compound. (Answer – $C_7H_6O_2$)

2) Find the empirical formula for a compound consisting of 63% Mn and 37% O . (Answer - MnO_2)

3) The empirical formula for vitamin C is $C_3H_4O_3$. Experimental data indicates that the molecular mass of vitamin C is 176. What is the molecular formula of vitamin C? (Answer – $C_6H_8O_6$)