STOICHIOMETRY CALCULATIONS WITH CHEMICAL FORMULAS AND EQUATIONS

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Introduction

The way we express different states of matter and the variation take place in its chemical composition is not confined to use in chemistry class or chemical lab; it can be seen widely in scientific world. Think about chemical symbols, formulas, and equations as the universal language of science, showing up not only in chemistry but also in fields as varied as engineering, agriculture, pharmacy, geology, physics, biolog and medical sciences. Now, let's dive a bit deeper into the heart of this linguistic marvel called stoichiometry. In stoichiometry, we master the art of balancing chemical equations and uncovering the precise numerical relationships between the starting materials (*reactant*) and the resulting yields (*product*) (Vaz Jr, 2023)(Danzer, 2007). Imagine you're in a bakery, and you have a recipe that tells you how much flour, sugar, and eggs you need to make the perfect cake. Stoichiometry is like that recipe; it helps scientists and students predict, manage, and enhance chemical reactions just like a baker would whip up a delectable cake. So, whether you're formulating new materials in a lab or making delicious treats in the kitchen, stoichiometry is your trusty guide to ensure everything turns out as planned (Valcárcel Cases et al., 2018).

The term "stoichiometry" finds its roots in ancient Greek, where "stoicheion" (translated as element) and "metron" (interpreted as measure) come together to form its name. This linguistic history beautifully illustrates the core concept of stoichiometry, which is all about measuring and quantifying the elements and compounds that play a role in a chemical reaction. To put it simply, stoichiometry helps chemists figure out the exact amounts of starting materials needed, and the quantities of products generated. Stoichiometric calculations are the foundation upon which the entire building of chemical science stands, forming an essential scaffolding for comprehending and foretelling the consequences of chemical transformations. Imagine stoichiometry as the GPS of the chemical world, charting the precise course of atoms and molecules in their intricate choreography. It's not an overstatement to declare that stoichiometry holds a pivotal role in the realm of chemistry, not only by

unravelling the theoretical mysteries of reactions but also by providing a guiding star for practical applications across diverse industries (Mosher et al., 2023). Consider the example of pharmaceuticals: here, stoichiometry acts as a skilled pharmacist, ensuring that every ingredient in a medication plays its role in harmony, resulting in safe and effective drugs (Fahlman, 2023). Similarly, in the realm of energy production, stoichiometric insights optimize the combustion of fuels, like a master chef perfecting a recipe, ensuring maximum energy output with minimal waste. In essence, stoichiometry is the chemist's trusted companion, illuminating the path from the initial mixture of ingredients to the final product, whether it's a life-saving medicine or a sustainable energy source.

Molecular mass /Weight and Molar Mass:

Molar mass refers to the weight of one mole of a substance, usually stated in g/mol. It is same in numerical value to the molecular mass of a substance measured in amu. In chemical computations, molar mass is employed to establish the correlation with the mass of a compound and the quantity of moles it encompasses. As an illustration, the water (H_2O) is approximately is 18 g/mol, indicating that a single mole of water molecules possesses a mass of 18 amu.

The Mole:

The smallest amount of matter that can be consistently manipulated havinng an incredibly vast number of atoms. Consequently, in any practical scenario, we encounter substantial quantities of atoms, making it advantageous to have a unit for effectively expressing such large numbers.

The concept of quantifying specific quantities with units has a long history. Familiar units like a dozen (12 units) are well-known. In the International System of Units (SI), the mole (mol) is the standardized unit for measuring quantity of a substance. The amount containing the same entities as atoms present in 0.012 kg of pure carbon-12, even the smallest amount of matter has an astonishing number of atoms. In practical scenarios, dealing with these microscopic building blocks requires a convenient way to describe immense numbers of atoms, emphasizing the importance of the mole as a fundamental unit of measurement (Donald A. McQuarrie, Peter A. Rock, 2010).

It is accurately said as the quantity of compound containing an equivalent number of entities, be they atoms, molecules, as found in precisely 0.012 kilograms of pure carbon-12.

$$1 mole = 6.02214179 \times 10^{23} \ particles$$

Avogadro's number, approximately 6.0223×10^{23}, is a tribute to the remarkable contributions of Amedeo Avogadro (1776–1856) to the field of chemistry. Avogadro's number defines what we call 'the mole'—a special unit that signifies a fixed quantity of stuff, with each piece of stuff having its own unique identity. Think of it this way: Just as we casually talk about a dozen eggs or a pair of aces in a deck of cards, we use the term 'a mole' to describe a certain number of atoms, molecules, ions, electrons, or any other tiny particles you can imagine. Imagine helium for a moment. It exists as individual helium atoms, so when we talk about 'one mole of helium,' we're actually talking about 6.0223×10^{23} helium atoms all hanging out together. Now, consider hydrogen, diatomic molecules. So, it means 6.0223×10^{23} H_2 molecules, which also amounts to twice that number, $2(6.0223 \times 10^{23})$, of individual H atoms.

Here's the magical part: Each type of atom, molecule, or ion has its own special weight, a unique characteristic mass. And because of this, 01 mole of any compound possesses a precise weight, no matter where you find it. This concept is vital in countless chemistry and science calculations. As mole is the quantity of particles present in 12 g of ^{12}C. The atomic mass unit, is established as 1/12th of a single ^{12}C atom's mass. This presents a straightforward yet potent principle: The mass of one mole of atoms from any pure element, measured in grams, precisely equals the element's atomic weight in amu. Therfore we termed the 'molar mass,' is denoted in units such as grams per mole (g/mol) or g mol^{-1}.

Example 1: How many amu in 01 g of ^{12}C

$$\underline{?}\ \text{amu} = 1.000\ \text{g}\ ^{12}\text{C atoms} \times \frac{1\ \text{mol}\ ^{12}\text{C}}{12\ \text{g}\ ^{12}\text{C atoms}} \times \frac{6.022 \times 10^{23}\ ^{12}\text{C atoms}}{1\ \text{mol}\ ^{12}\text{C atoms}} \times \frac{12\ \text{amu}}{^{12}\text{C atom}}$$

$$= 6.022 \times 10^{23}\ \text{amu}$$

$$1\ \text{g} = 6.022 \times 10^{23}\ \text{amu} \quad \textit{or} \quad 1\ \text{amu} = 1.660 \times 10^{-24}\ \text{g}$$

Molar Mass:

Molar mass, a vital concept in chemistry, represents the mass of a single mole of a substance and is typically represented in g/mol. This value is exactly equivalent to the

molecular mass, which is measured in amu for compounds. Molar mass plays a crucial role in chemical computations, helping us bridge the gap between mass and moles. Let's dive into this concept with a practical example. Imagine a glass of water, H_2O, a fundamental compound we encounter daily. Its molar mass is approximately 18 g/mol. This means that if we were to gather one mole of water molecules, we'd have a hefty 18 grams of water right there.

Chemists streamline calculations using a unit called a 'mole.' In essence, a mole is the amount of compound with a mass, measured in g, exactly same as to thier formula mass. Denoted by 'mol,' when benzene (C_6H_6) has a formula mass of 78.11, its molar mass is readily identified as 78.11 g/mol. (Kenneth W. Whitten, Raymond E. Davis, Larry Peck, 2010).

Now, the magic happens when we need to switch between mass and moles in chemical calculations. Take benzene as an example again, with its formula mass of 78.11. This indicates that there are precisely 78.11 grams in one mole of C_6H_6. This insight provides us with two versatile unit conversion factors:

$$\frac{1mol\,C_6H_6}{78.11g\,C_6H_6}=1, \qquad or \qquad \frac{78.11g\,C_6H_6}{1mol\,C_6H_6}=1$$

We can use a special number to switch between grams and moles when dealing with substances like C_6H_6. It's like a magical bridge. If you have grams and want moles, you can use it one way, and if you have moles and want grams, you can use it the other way around. For example, let's say you have 100 g of benzene, and you want to figure out how many moles that is. You start with what you know, which is the 100 g, and then you use this special number to find the answer, which is the moles.

$$\left(100\,g\,C_6H_6\right)\times\frac{1mol\,C_6H_6}{78.11g\,C_6H_6}=1.280\,mol\,C_6H_6$$

Note that the outcome is displayed with precision up to three significant digits. Furthermore, you have the option to determine the substance's mass when you have a specific quantity of moles at your disposal.

Example 2: Argon (Ar) gas is extracted from the air on an industrial scale. When we look at dry air, it contains a tiny 1.0 mole% of Argon, a whopping 78 mole% of Nitrogen (N_2), and a significant 21 mole% of Oxygen (O_2). Now, the question is,

how many kilograms of air do we need to extract just one kilogram of Argon? Ar has a mass of 40 amu, while Nitrogen weighs in at 14 amu.

Solution:

$$N_2 = 78 \times 28 = 2184\ grams$$
$$O_2 = 21 \times 32 = 672\ grams$$
$$Ar = 1 \times 40 = 40\ grams$$
$$2896\ grams$$

$$g\ of\ air = \left(\frac{2896\ g\ air}{40\ g\ Ar}\right)(1000\ g\ Ar) = 72400\ g = 72.4\ kg$$

Example 3: You have a 30.0 gram sample of a unknown substance which consist of carbon (C), hydrogen (H), and oxygen (O). When you burn it (combustion), you get 25 g of CO_2 and 30 g of H_2O. Calculate the oxygen molecules were used from the air during this process? Also, explain the way we capture CO_2 and H_2O in this combustion experiment.

Solution:

$$Organic\ compound + O_2 \rightarrow CO_2 + H_2O$$
$$30\ g + Xg \rightarrow 25\ g + 30\ g$$

Total Material Balance:

$$Total\ mass\ of\ reactants = Total\ mass\ of\ product$$

Thus **X = 25 g**

$$Molecule\ of\ X\ or\ O_2\ from\ air = (25\ g\ O_2)\left(\frac{1\ mol\ of\ O_2}{32\ g\ of\ O_2}\right)\left(\frac{6.02\times10^{23}\ Molecule\ of\ O_2}{1\ mol\ of\ O_2}\right) = 4.8\times10^{23}\ molecules$$

OR

$$g\ of\ C = (25\ g\ CO_2)\left(\frac{12\ g\ C}{44\ g\ CO_2}\right) = 6.82\ g\ of\ C$$

$$g\ of\ H = (30\ g\ H_2O)\left(\frac{2\ g\ H}{18\ g\ H_2O}\right) = 3.3\ g\ of\ H$$

$$g\ of\ O_2 = (30\ g\ of\ compound) - (6.82\ g\ C) - (3.3\ g\ H)$$

$$g\ of\ O_2\ in\ sample = 19.88\ g$$

$$g\ of\ O_2\ in\ product\ (H_2O\ and\ CO_2) = (25\ g\ CO_2)\left(\frac{32\ g\ O_2}{44\ g\ CO_2}\right) + (30\ g\ H_2O)\left(\frac{16\ g\ O_2}{18\ g\ H_2O}\right) = 44.85\ g$$

$$g\ of\ O_2\ from\ air = g\ of\ O_2\ in\ product - g\ of\ O_2\ in\ Sample = 44.8\,g - 19.88\,g$$

$$O_2\ molecules = (25\,g\,O_2)\left(\frac{1\,mol\ of\ O_2}{32\,g\ of\ O_2}\right)\left(\frac{6.02\times10^{23}\ molecules\ of\ O_2}{1\,mol\ of\ O_2}\right) = 4.8\times10^{23}\ molecules$$

Upon burning a sample with ample oxygen, the resulting water and carbon dioxide traverse chambers containing various substances. Magnesium perchlorate absorbs the water, and the subsequent chamber sees sodium hydroxide interacting with carbon dioxide. Evaluating the mass increase of magnesium perchlorate and sodium hydroxide measures the quantities of water and CO_2 produced during combustion.

Example 4: Imagine you're in an exam hall with dimensions of 80 m in length, 75 m in width, and 50 m in height. Now, let's figure out the amount of carbon dioxide (CO_2) present in kg. We know that the concentration of CO_2 in this room is 0.04% by volume, and the temperature (T) is 298 K, with the gas constant (R) being 8.314 J mol $^{-1}$ K^{-1}. The pressure (P) is 101325 Pascals, where 1Pa = 1N/m^2.

Method 1:

$$P = 10^5\ Pa$$
$$V = 80\,m\times75\,m\times50\,m = 300000\ m^3$$
$$R = 8.314\,J\,mol^{-1}K^{-1}\quad T = 298\,K$$
$$n = moles\ of\ air\ in\ the\ room = ?$$
$$PV = nRT \Rightarrow n = \frac{PV}{RT} = \frac{101325\ Pa\times300000\ m^3}{8.314\,Pa\,m^3\,mol^{-1}K^{-1}\times298\,K} = 1.21\times10^7\ mol\ of\ air\ in\ the\ room$$
$$grams\ of\ CO_2 = (1.21\times10^7\ mol\ of\ air)\times\left(\frac{0.04\,mol\,CO_2}{100\,mol\ air}\right)\times\left(\frac{44\,g\,CO_2}{1\,mol\,CO_2}\right)\times\frac{1kg}{1000\,g} = 216\,kg$$

Method 2:

$$grams\ of\ CO_2 = (300000\,m^3)\times\left(\frac{100\,L}{1m^3}\right)\times\left(\frac{0.04\,L\,CO_2}{100\,L\,air}\right)\times\left(\frac{1\,mol\,CO_2}{2445\,L\,CO_2\ at\ 298\,K}\right)\times\left(\frac{44\,g}{1\,mol\,CO_2}\right)\times\left(\frac{1kg}{1000\,g}\right) = 215\,kg$$

Writing a Balance Chemical Equation:

Creating balanced chemical equations stands as a core skill within the realm of chemistry. These equations serve as precise portrayals of chemical reactions, effectively illustrating the amound and types of both the initial substances and the resulting compounds. The significance of balanced chemical equations in the field of

chemistry cannot be overstated. They play a pivotal role for a variety of compelling reasons:

1. *Conservation of Mass:* The conservation of mass, a cornerstone of chemistry, asserts that matter remains unaltered in quantity during chemical reactions. It firmly states that matter's inherent nature is persistence, as it can neither be conjured into existence nor obliterated. When we skilfully construct balanced chemical equations, we are meticulously orchestrating a symphony where the combined mass of the starting materials, referred to as reactants, harmoniously converges with the mass of the newly formed substances, aptly termed products. Thus, we're not creating matter; we're choreographing its elegant dance of transformation.
2. *Stoichiometry:* Balanced chemical equations are like treasure maps for chemists, revealing the hidden secrets of mole ratios in a chemical metamorphosis. These ratios, akin to magical incantations, unveil the precise quantities of substances needed or produced during the enchanting dance of atoms and molecules. For any experimental alchemist or aspiring soothsayer, this knowledge is indispensable, for it empowers them to wield their reactions with precision and foresee their mystical outcomes.
3. *Predicting Products:* A well-orchestrated balanced chemical equation acts as a crystal ball, foretelling the future of a chemical reaction. It offers valuable insights into the substances that will emerge from the alchemical cauldron and the precise quantities in which they shall manifest under specific enchanting conditions.
4. *Quantitative Analysis:* Balanced equations are the alchemical keys to the realm of quantitative analysis. They empower practitioners to gauge the concentration of elixirs, divine the yield of reactions, and measure the efficiency of arcane chemical processes.
5. *Reaction Understanding:* Balanced equations provide a clear picture of chemical reactions. They help students to see how chemical reacts and transform into products.
6. *Communication:* Balanced equations transcend linguistic barriers, serving as a universal tongue that unites chemists worldwide. They foster seamless communication, ensuring that scientists across the globe can comprehend and replicate experiments and rituals with unwavering accuracy.

There are different methos used for balancing a chemical equation, Some of the most commonly utilized methods include(Brown, Lawrence S., 2011):

a) **Trial-and-Error Technique:** This approach is quite simple. You tweak the numbers in front of the chemicals in the equation until the count of atoms for every compound matches on either side of the chemical reaction.
b) **Redox Balancing:** In redox reactions, which involve electron exchange, the half-reaction method is applicable. This technique involves dividing the overall reaction into oxidation and reduction reactions. Subsequently, the atoms on either side of reaction are balanced, and charges are individually balanced. Finally, the half-reactions are combined to yield the overall reaction.
c) **Electron Transfer Balancing:** This method is used for redox reactions, and again we split the overall reaction into oxidation and reduction. During this kind of reaction, the oxidation state

of element changes and by putting suitable number of electrons to balance half reaction. Finally, both reactions are added to get the overall balance chemical equation.

d) **Mathematical Approach:** This is a more straightforward way to balance a very complex reaction in a short time. Here we make a set of equations to represent conversion of mass of each element in the reaction. Then using mathematical skill to solve these equations simultaneously to find the value of variables and coefficient for every element and compounds which ultimately gives us the balance chemical equation.

Algebraic Method:

The algebraic approach to balancing chemical equations is a valuable technique. It entails creating a set of linear equations to express the principle of mass conservation for every element within the reaction. This method proves especially handy when dealing with intricate chemical equations, as it offers a systematic solution instead of relying on trial-and-error or visual inspection. Now, let's break down the algebraic method into simple steps for a clearer understanding:

The algebraic method to balance a chemical equation is a useful method. Using this method, we can easily balance a very complex reaction within two minutes and in similar way we can also solve or balance a simple reaction in two minutes, and this is the only advantage and disadvantage of this mathematical approach. Here we supposed variables for each element in reactant and products and then we set linear equations to represent the main conversion of mass (reactant into product) in given reaction. Now we assume the value of one variable to find out the values of other variables. Then we solve this linear equation to find out the value of other variables (elements). The following is the schematic for easily understanding this method.

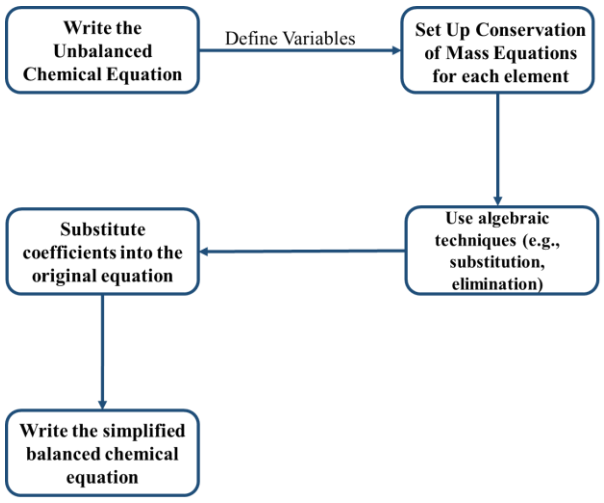


Figure 1. Breakdown of algebraic methods into simple steps

Example 5:

$$CaSO_4 + CH_4 + CO_2 \rightarrow CaCO_3 + S + H_2O$$
$$aCaSO_4 + bCH_4 + cCO_2 \rightarrow dCaCO_3 + eS + fH_2O$$

Solution:

Assume a = 1, then e = d = 1

Mass balance:

$Ca: \ a = d$

$S: \ a = e$

$O: \ 4a + 2c = 3d + f$

$C: \ b + c = d$

$H: \ 4b = 2f$

$$\Rightarrow \begin{bmatrix} 4 + 2c = 3 + f \\ Since, \\ b + c = 1 \rightarrow c = 1 - b \\ 4 + 2(1-b) = 3 + f \\ and, \\ f = 3 + 2b \\ b = 3/4 \\ c = 1 - 3/4 = 1/4 \\ f = 6/4 \end{bmatrix}$$

So,

$$CaSO_4 + 3/4\,CH_4 + 1/4\,CO_2 \rightarrow CaCO_3 + S + 6/4\,H_2O$$
$$4CaSO_4 + 3CH_4 + CO_2 \rightarrow 4CaCO_3 + 4S + 6H_2O$$

How do we balance charge in the algebraic method?

$$aMnO_4^- + bH^+ + cFe^{2+} \rightarrow dMn^{2+} + eFe^{3+} + fH_2O$$

Mass balance:

$For: \ Mn \rightarrow a = d$

$For: \ Fe \rightarrow c = e$

$For: \ O \rightarrow 4a = f$

$For: \ H \rightarrow b = 2f$

Charge balance: $-a + b + 2c = 2d + 3e$

Assuming $a = 1$, *then* $\rightarrow$

$$-1 + b + 2c = 2 + 3e$$
$$-1 + 2f + 2e = 2 + 3e$$
$$-1 + 8 - 2 = e$$
$$e = 5, \ c = 5, \ a = 1, \ d = 1, \ f = 4, \ b = 8$$

$$\mathbf{MnO_4^- + 8H^+ + 5\,Fe^{2+} \rightarrow Mn^{2+} + 5Fe^{3+} + 4H_2O}$$

Example 6: Apply the algebraic way to balance the equation:

$$AsO_3^{3-}{}_{(aq)} + Br_{2(aq)} + OH^-{}_{(aq)} \rightarrow AsO_4^{3-}{}_{(aq)} + Br^-{}_{(aq)} + H_2O_{(l)}$$

Solution:

$$aAsO_3^{3-} + bBr_2 + cOH^- \rightarrow dAsO_4^{3-} + eBr^- + fH_2O$$

Material Balance shows		Charge balance
As:	a = d	–3a – c = –3d–e
O:	3a + c = 4d + f	
Br:	2b = e	
H:	c = 2f	

$$\text{Assuming:} \quad a=1, \Rightarrow d=1$$

$$3+c=4+f$$

$$c=2f$$

$$3+2f=4+f \Rightarrow f=1$$

$$c=2$$

$$-3-2=-3-e \Rightarrow e=2, \quad and \quad b=1$$

$$a=1, \quad b=1, \quad c=2, \quad d=1, \quad e=2, \quad f=1$$

$$AsO_3^{3-} + Br_2 + 2OH^- \rightarrow AsO_4^{3-} + 2Br^- + H_2$$

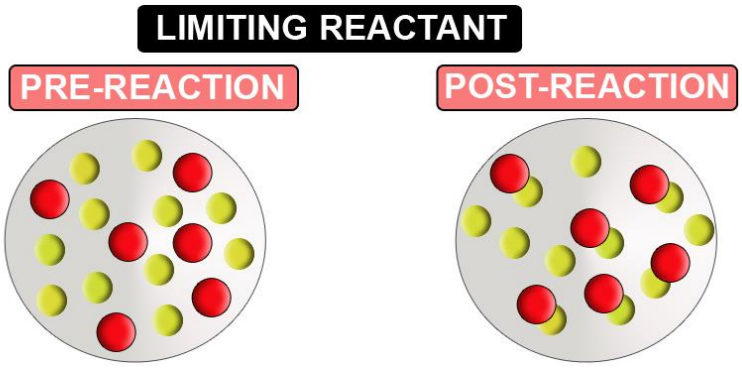


Figure 2. Diagrammatic representation of limiting reactant pre and post reaction

Limiting Reactant:

The limiting reactant has a prime importance in chemical reactions as well as in chemical industry as it decides the amount of product generated during any chemical process. The limiting reactant control the amount of yeild produced in a balance chemical equation. The other reactant which remains unreacted once the reaction complete is known as excess reactant. We can understand the concept by considering the following analogy:

Assume you are baking cookies. You have a limited supply of flour, sugar, and chocolate chips. These are the ingredients for your cookies. Flour and sugar are the limiting reactants here because they are the ones you run out of first. Once you've used up all your flour and sugar, you can't make any more cookies, even though you might still have plenty of chocolate chips left. The flour and sugar are like the limiting reactants, while the chocolate chips are the excess reactant. They remain unused because there's nothing left to react with once the flour and sugar are exhausted (Theodore Brown, H. LeMay, Bruce Bursten, Catherine Murphy, Patrick Woodward, 2012).

Example 7: Aluminum chloride, $AlCl_3$, plays a crucial role in various industries such as rubber production, lubricant manufacturing, wood preservation, and paint formulation. It can be synthesized through a simple process: the direct combination of aluminum and chlorine:

$$2Al_{(s)} + 3Cl_{2(g)} \rightarrow 2AlCl_{3(s)}$$

To better understand this reaction, let's explore an example. Imagine you have 3.5 grams of aluminum (Al) and 5.2 grams of chlorine gas (Cl_2) available for this reaction. Our goal is to determine the limiting reactant, find out:

a) Which of the two reactants is the limiting one?
b) How much of the excess reagent remains unused?
c) What quantity of product will be produced?

Solution:

In every stoichiometric calculation, the first crucial step involves finding the quantity of moles for each of the substances taking part in the reaction. This step is as fundamental as measuring ingredients for a recipe before cooking them, ensuring that you have the right amounts of each reactant, just like a chef measures out flour, sugar, and eggs before making a cake.

$$Moles\,of\ Al = (3.5g\ Al\ ) \times \left(\frac{1mol\ Al}{26.98g\ Al} \right) = 0.1297\,mol\ Al$$

$$Moles\,of\ Cl_2 = \left(5.2\text{g}\,Cl_2\right)\left(\frac{1\ \text{mol}\ Cl_2}{71\ \text{g}\ Cl_2} \right) = 0.0732\,mol\,Cl_2$$

Observing the balanced equation, we notice that when two moles of Aluminum react, they yield an equal amount of two moles of $AlCl_3$. So, when we start with 0.1297 moles of Aluminum, it gives us precisely 0.1297 moles of $AlCl_3$. In a similar fashion,

if we consider three moles of chlorine, they produce two moles of $AlCl_3$. Thus, starting with 0.0732 moles of Cl_2, we get 2/3 × 0.0732 moles of $AlCl_3$, which equals 0.049 moles of $AlCl_3$. Now, what's interesting is that Cl_2, with its 0.049 moles of $AlCl_3$ production, turns out to be the **limiting reagent** because it produces the least amount of $AlCl_3$.

Now, Al is the **excess reactant**, so we can determine its quantity by:

3 mol. of Cl_2 reacts with 2 mol. of Al

Hence, when you have 0.073 moles of Cl2, it will combine with 0.049 moles of aluminum (which is 2/3 of 0.073 mol)

Al = 0.13 mol.

Therefore, the remaining amount of Al or the amount of excess reactant = 0.13 – 0.049 = 0.081 mol.

Remaining Amount of Al = mol Al x molar mass of Al

$$=\left(0.081 mol\ Al\right)\times\left(\frac{27\,g\ Al}{1 mol\ Al}\right)=2.2\,g\ Al_{(s)}$$

Lastly, the g of product produced can be found as:

The mol of product calculated using the limiting reactant are 0.049 mol of $AlCl_3$

To convert it into grams.

Amount of $AlCl_3$ produced in the reaction :

$$=\left(0.049 mol\ AlCl_3\right)\times\left(\frac{133.5\,g\ AlCl_3}{1 mol\ AlCl_3}\right)=6.54\,g\ AlCl_{3(s)}$$

A Fast Way to Identifiy Limiting Reactants:

A rapid approach to identify a limiting reactant involves determining its moles and dividing each reactant's moles by its reaction coefficient in the balanced chemical reaction. The reactant with the lowest result is the limiting reactant. This method streamlines limiting reactant identification by focusing on mole ratios.

Example 8: In the thermite reaction, either 20 g of $Al_{(s)}$ or 52 g of $Fe_2O_{3(s)}$ served as the limiting reactant. These masses equate to 0.325 moles of Fe_2O_3(s) and 0.740 moles

of $Al_{(s)}$. Utilizing the coefficients in the balanced chemical reaction, let's analyze their reaction.

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

Solution: To ascertain whether either of these substances is a limiting reactant, calculate the moles for each species and divide by its respective stoichiometric coefficient.

0.740 moles Al /2 = 0.37 mol

and 0.325 moles of Fe_2O_3/ 1 = 0.325 mol

As the moles of $Fe_2O_{3(s)}$ divided by its stoichiometric coefficient are fewer than the moles of Al(s) divided by its stoichiometric coefficient, we determine that $Fe_2O_{3(s)}$ serves as the limiting reactant. This approach proves beneficial in solving problems with more than two reactants.

When the computed product quantity remains constant for distinct reactants, it implies you've determined the theoretical yield using both reactants, resulting in equivalent yields. In this scenario, neither reactant serves as the limiting reactant, as both can fully react to yield the same product quantity. The limiting reactant, which dictates the maximum product formation, is the one entirely consumed first, thereby restricting the reaction extent. When both reactants have the same theoretical yield of the product, it means that both reactants can react completely, and there is no limitation imposed by either of them. In summary, if the calculated amount of product is the same when considering both reactants, neither reactant is the limiting reactant, and both can be considered as "equally limiting" in the sense that they both contribute to the maximum possible yield of the product.

Theoretical, Actual and Percentage Yield:

When chemical reactions take place, we can anticipate the amounts of substances created by using the connection between the starting materials and the end products, which is explained through chemical equations. Nevertheless, in actual chemical reactions, things don't always go as planned because of a variety of factors.

Theoretical Yield:

Theoretical yield, in chemistry, describe the perfect quantity of yeilds expected from a reaction, considering the a balance chemical reaction. It's what we'd get if the reaction ran perfectly without any losses or issues. You can calculate it with this formula:

TY = (moles of limiting reactant) x (molar mass of product)

This represents the product yield obtained when the limiting reagent fully reacts, as shown in our earlier example.

Actual Yield:

The actual yield represents the real-world quantity of product obtained in a chemical reaction, considering practical limitations and inefficiencies. Factors such as incomplete reactions, side reactions, purification-related losses, impurities, and unexpected occurrences often result in the actual yield being less than the theoretical yield. Experimentally, the actual yield (AY) is determined through measurements.

Percentage Yield:

The performance of a chemical reaction and the corelation between actual and theoretical yields are gauged by the percent yield. Calculated with a specific formula, the percent yield quantifies the proportion of actual yield to theoretical yield.

$$Percentage\ yield = \left(\frac{Actual\ Yield}{Theoretical\ Yield} \right) \times 100$$

Calculating the percentage yield allows chemists to quantify the success of a reaction and identify areas for improvement in reaction efficiency. A percentage yield less than 100% indicates that the reaction did not proceed to completion or that some product was lost, or some undesired by-products were formed.

Example 9: A 30.5 g zinc (Zn) sample is reacted with higher quantity of nitric acid (HNO_3) and produces 65.2 g of Zinc nitrate ($Zn(NO_3)_2$).

$$Zn_{(s)} + 2\ HNO_{3(aq)} \rightarrow Zn\left(NO_3\right)_{2(aq)} + H_{2(g)}$$

Find out the theoretical yield, the actual yield, and the percentage yield.

Solution:

The theoretical yield of $Zn(NO_3)_2$ is;

$$Theoretical\ yield = (30.5\ g\ Zn) \times \left(\frac{1\ mol\ Zn}{65.38\ g\ Zn}\right) \times \left(\frac{1\ mol\ Zn(NO_3)_2}{1\ mol\ Zn}\right) \times \left(\frac{189.36\ g\ Zn(NO_3)_2}{1\ mol\ Zn(NO_3)_2}\right)$$

$$= 88.34 g\ Zn(NO_3)_2$$

The actual yield of $Zn(NO_3)_2$ is the quantity produced, which, as mentioned, is 65.2 grams.

The percentage yield is given by:

$$\%\, yield = \left(\frac{actual\ yield}{theoretical\ yield}\right) \times 100 = \left(\frac{65.2}{88.34}\right) \times 100 = 73.8\ \%$$

Hence, we can conclude that the reaction has achieved approximately three-fourths of its maximum potential yield.

Empirical and Molecular Formulas:

Within the realm of chemical calculations, understanding the composition of compounds is a fundamental aspect of chemical analysis. Chemical formulas serve as concise representations of the elements present within a compound, as empirical and molecular formulas.

Empirical Formulas:

Empirical formulas represent the simplest whole-number ratio of atoms within a compound. These formulas give us a basic knowledge about comparable proportions of various elements in a compound and minimize the complexity of multiple atoms of the same element in a molecule. The empirical formula can be determined using experimentation and analysis. For example, molecular formula of Glucose is $C_6H_{12}O_6$. The Simplest or empirical formula would be CH_2O as it is showing the simple whole-number ratio of carbon (C), hydrogen (H), and oxygen (O) atoms.

Molecular Formulas

The molecular formulas give us a detailed representation of a compounds composition by representing the exact number and types of atom in compound. These describe an accurate detail of a compound which include number of atoms and their arrangement (Donald A. McQuarrie, Peter A. Rock, 2010). As we see in our previous example,

that Glucose has $C_6H_{12}O_6$ formula, there are 06 carbon, 12 hydrogen, and 06 oxygen atoms. Molecular formulas are important if we want to understand the exact configuration of a compound. The molecular formulas can easily be calculated from empirical formula by using following equation.

Molecular Formula = n × Empirical Formula

Here in "n" is factor which can be determined as

n = molecular formula mass / empirical formula mass

For Example:

Let the Benzene, having empirical formula CH. Its molecular formula is C_6H_6.

Molecular formula mass of Benzene = 78 g/mol

Empirical formula mass of Benzene = 13

So n will be equal to 78/13 = 6

In this case, Molecular Formula for Benzene (CH) = 6 × Empirical Formula (CH)

= C_6H_6

Example 10: Upon complete combustion of 0.50 g of ascorbic acid commonly known as vit-C having C, H, and O atoms, resulting in 0.75 g of CO_2 and 0.205 g of H_2O, deduce the empirical formula. With atomic masses: C (12 amu) and O (16 amu), if the molecular mass is 176 amu, establish the molecular formula.

Solution:

$$\text{g of C} = (0.75\ \text{g } CO_2)\left(\frac{12\ \text{g C}}{44\ \text{g } CO_2}\right) = 0.204\ \text{g of C}$$

$$\text{g of H} = (0.205\ \text{g } H_2O)\left(\frac{2\ \text{g H}}{18\ \text{g } H_2O}\right) = 0.022\ \text{g of H}$$

$$g\ of\ O = (0.50\ g\ of\ compound) - (0.204\ g\ C) - (0.022 g\ H)$$

$$g\ of\ O = 0.274\ g$$

$$\text{Mole of C} = (0.204\ \text{g C})\left(\frac{1\ mole\ \text{C}}{12\ \text{g C}}\right) = 0.017\ mol\ of\ \text{C}$$

$$Mole\ of\ \mathrm{H} = (0.022\ \mathrm{g\ H})\left(\frac{1\ mole\ \mathrm{H}}{1\ \mathrm{g\ H}}\right) = 0.022\ mol\ of\ \mathrm{H}$$

$$Mole\ of\ \mathrm{O} = (0.274\ \mathrm{g\ O})\left(\frac{1\ mole\ \mathrm{O}}{16\ \mathrm{g\ O}}\right) = 0.017\ mol\ of\ \mathrm{O}$$

$$0.017\ mole\ of\ \mathrm{C} \cong 0.022\ mole\ of\ \mathrm{H} \cong 0.017\ mole\ of\ \mathrm{O}$$

$$dividing\ by\ lowest\ \text{i.e}0.017$$

$$1\ mole\ of\ \mathrm{C} \cong 1.3\ mole\ of\ \mathrm{H} \approx 1\ mole\ of\ \mathrm{O}$$

$$multiply\ by\ lowest\ 3\ to\ get\ whole\ number$$

$$3 mole of\ C \cong 4 mole of\ H \approx mole of\ O$$

So the empirical formula of the comound will be $C_3H_4O_3$

The molecular mass is given i.e. 176 and the empirical formula mass is 88,

so the molecular formula must be $\frac{176}{88} = 2$ times the empirical formula.

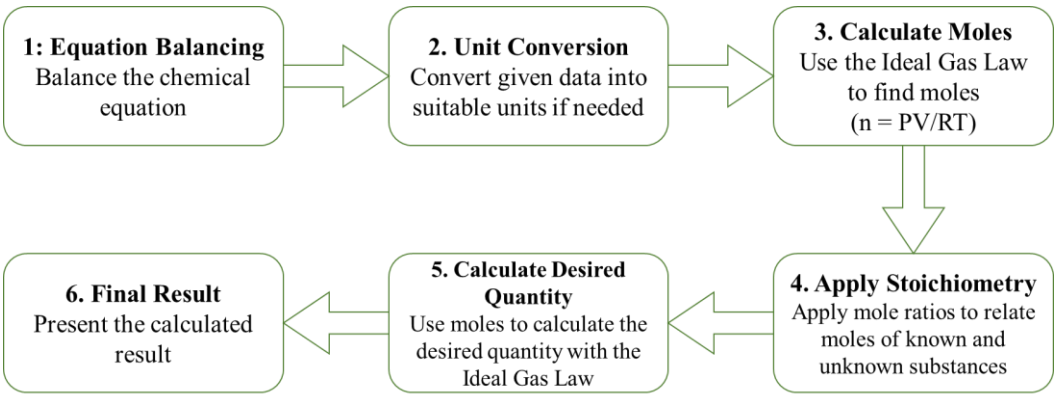
Thus, the molecular formula is $= 2(C_3H_4O_3) = C_6H_8O_6$.

Gas Stoichiometry:

Chemical stoichiometry also the reactants and products chemical reactions in gaseous phase. While reactions involving gases share similarities with those involving solids and liquids, the incorporation of the Ideal Gas Law (PV=nRT) distinguishes them. Utilizing this law, we can compute the quantity of gas molecules present when armed with information on volume, pressure, and temperature(Andrew Burrows, John Holman, Simon Lancaster, Tina Overton, 2017).

Laboratory processes often encompass the formation or reaction of gases, necessitating chemists' competence in quantifying gaseous reactants and products, akin to their treatment of solids or solutions. Additionally, many crucial industrial reactions occur gaseous state. Gases readily combine, facilitate heating or cooling, and can be conveniently transported within manufacturing facilities through basic pumps and plumbing (Atkins, 2006).

Stoichiometric calculations for gas-involved reactions commonly involve the Ideal Gas Law Below is a comprehensive guide to executing stoichiometric computations.



Here's is the illustrattion steps:

Example 11: In the reaction $2H_2 + O_2 \rightarrow 2H_2O$, 5.0 moles of hydrogen gas (H_2) react with high amount of O_2 gas Calculate the volume of water vapor (H_2O) produced at 25°C and 1.00 atm.

Solution

Step 1: Balance the equation: $2H_2 + O_2 \rightarrow 2H_2O$.

Step 2: Convert temperature to Kelvin: 25 °C + 273.15 = 298.15 K.

Step 3: Compute the mol of H_2:

$$n=\frac{(PV)}{(RT)} \rightarrow n=\frac{(1atm)\times(1L)}{(0.0821L{\cdot}atm/(mol{\cdot}K)\times 298.15K)} \rightarrow n\approx 0.0406\,moles\,of\ H_2$$

Step 4: Apply stoichiometry:

Using the balanced equation, 2 moles of H_2 produce 2 moles of H_2O.

Step 5: Calculate the volume of H_2O:

Since 2 moles of H_2 produce 2 moles of H_2O, and we have 0.0406 moles of H_2, we will also have 0.0406 moles of H_2O.

Now, applying PV=nRT to find Vol:

$$n=\frac{(PV)}{(RT)} \rightarrow 0.0406\,moles=(1.00\,atm)\times\frac{V}{(0.0821L{\cdot}atm/(mol{\cdot}K)\times 298.15K)} \rightarrow V\approx 1.73L.$$

So, approximately 1.73 L of water vapor are produced in the reaction.

Gas Stoichiometry Principles:

Gas stoichiometry relies heavily on gas properties, especially molar volume, in elucidating the quantitative relationships between reactants and products during chemical reactions involving gases. Here's how these gas properties come into play (Ralph H. Petrucci, Carey Bissonnette, F. Geoffrey Herring, 2007):

- Molar Volume (V_m): Molar volume signifies the space occupied by 01 mol of a gas under certain T and P, often denoted in L/mol. Particularly notable at STP, approximately 22.4 L/mol, it simplifies conversions between moles and volume in gas stoichiometry. For instance, having 2 moles of a gas at STP translates to a volume of 44.8 L (2 moles * 22.4 L/mol).
- Ideal Gas Law: interrelates pressure (P), volume (V), moles of substance (n), and temperature (T) for a gas. It proves valuable for deducing unknown gas properties or calculating the quantity of gas involved in a chemical reaction. For example, it aids in determining the moles of gas generated in a reaction when furnished with volume, pressure, and temperature data.
- Stoichiometry Ratios: In the context of chemical reactions, balanced chemical equations offer stoichiometric coefficients that essentially delineate the mole ratios governing reactants and products. These ratios become particularly pivotal in gas stoichiometry, aiding in establishing the connection between the reactants and products.
- Combining Gas Laws: Gas stoichiometry frequently necessitates the integration of various gas laws like Boyle's law ($P_1V_1 = P_2V_2$) or Charles's law ($V_1/T_1 = V_2/T_2$) with stoichiometric ratios to solve for hitherto unknown variables. For instance, Boyle's law can be employed to deduce the final volume of a gas when initial volume and pressure values are provided, and pressure undergoes alterations during a reaction.

Complex Stoichiometric Problems:

Below are the advanced stoichiometric problems involving multiple reactions and the combination of various stoichiometric principles, including mole ratios, reaction stoichiometry, and the Ideal Gas Law.

1- Multiple Reactions:

Example 12: In a complex chemical process, ammonia (NH_3) is produced rom nitrogen (N_2) and hydrogen (H_2). The reactions occur in two steps:

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)} \left(Formation\, of\ ammonia\right)$$
$$2NH_{3(g)} \rightarrow N_{2(g)} + 3H_{2(g)} \left(Decomposition\, of\ ammonia\right)$$

Suppose you start with 5.0 moles of N_2 and 15.0 moles of H_2. Calculate the final amount of ammonia and the remaining amounts of N_2 and H_2 after both reactions.

Solution:

Calculate the moles of NH_3 generated in the first reaction:

From the balanced equation, 1 mole of N_2 produces 2 moles of NH_3.

Moles of NH_3 formed = (5.0 moles of N_2)×(2 moles of NH_3 /1 mole of N_2) = 10.0 moles of NH_3.

Calculate the moles of NH_3 consumed in the second reaction:

From the balanced equation, 2 moles of NH_3 produce 1 mole of N_2.

Moles of NH_3 consumed = (10.0 moles of NH_3)×(1 mole of N_2 / 2 moles of NH_3) = 5.0 moles of N_2.

Calculate the moles of H_2 consumed in the second reaction:

From the balanced equation, 2 moles of NH_3 produce 3 moles of H_2.

Moles of H_2 consumed = (10.0 moles of NH_3)× (3 moles of H_2 / 2 moles of NH_3) = 15.0 moles of H_2.

Calculate the remaining moles of N_2:

Initial moles of N_2 – Moles of N_2 consumed = 5.0 moles – 5.0 moles = 0 moles.

Calculate the remaining moles of H_2:

Initial moles of H_2 – Moles of H_2 consumed = 15.0 moles – 15.0 moles = 0 moles.

So, after both reactions, you have 0 moles of N_2 and 0 moles of H_2 remaining, and you have 10.0 moles of NH_3.

2- Combining Stoichiometric Principles:

Example 13: In the combustion of methane (CH_4), 1.00 mole of CH_4 interact with 2.00 moles of O_2 to generate CO_2 and H_2O. Calculate the volume of CO_2 produced at STP when 4.00 moles of CH_4 are burned completely.

Solution:

Determine the moles of O_2:

1 mole of CH_4 requires 2 moles of O_2.

Moles of O_2 needed = (4.00 moles of CH_4) × (2 moles of O_2 / 1 mole of CH_4) = 8.00 moles of O_2.

Use the Ideal Gas Law to find volume of CO_2 at STP:

Since 1 mole of any gas occupies 22.4 L

Vol of CO_2 = (8.00 moles) × (22.4 L/mol) = 179.2 L.

So, 179.2 L of CO_2 are produced when 4.00 moles of CH_4 are burned completely at STP.

3- Limiting Reactants and Percent Yield:

Example 14: In the synthesis of ammonia (NH_3), 4.00 moles of nitrogen (N_2) react with 12.0 moles of hydrogen (H_2) as below:

$$N_{2(g)} + 3H_{2(g)} \rightarrow 2NH_{3(g)}$$

a) Find the limiting reactant.

b) Compute the moles of NH_3.

c) If the reaction goes to completion under the given conditions (no excess reactants), calculate the actual moles of NH_3 produced.

d) The percent yield if 7.50 moles of NH_3 are obtained.

Solution:

a) To find out the limiting reactant, we need to compare the moles of NH_3 that can be produced from both N_2 and H_2.

From N_2: 4.00 moles of N_2 * (2 moles of NH_3 / 1 mole of N_2) = 8.00 moles of NH_3.

From H_2: 12.0 moles of H_2 * (2 moles of NH_3 / 3 moles of H_2) = 8.00 moles of NH_3.

Both N_2 and H_2 produce 8.00 moles of NH_3, so there is no limiting reactant; both N_2 and H_2 are in excess.

b) The maximum moles of NH_3 that can be produced are:

Moles of NH_3 produced = (4.00 moles of N_2) * (2 moles of NH_3 / 1 mole of N_2) = 8.00 moles of NH_3.

c) If the reaction goes to completion under the given conditions with no excess reactants:

Moles of NH_3 produced = (4.00 moles of N_2) * (2 moles of NH_3 / 1 mole of N_2) = 8.00 moles of NH_3.

So, if the reaction goes to completion, 8.00 moles of NH_3 will be produced.

d) To calculate the percent yield, use the formula:

Percent Yield = (Actual Yield / Theoretical Yield) * 100

Given that the actual yield is 7.50 moles of NH_3 and the theoretical yield is 8.00 moles (as calculated in part c):

$$Percent\,Yield = \left(\frac{7.50\,moles}{8.00\,moles}\right) \times 100 = 93.75\%$$

The percent yield is 93.75% when 7.50 moles of NH_3 are obtained.

4- Gas Stoichiometry with Volume and Temperature Changes:

Example 15: A 5.00-liter container is initially filled with hydrogen gas (H_2) at 27°C and 2.00 atm pressure. It reacts with excess oxygen gas (O_2) to form water vapor (H_2O):

$$2H_{2(g)} + O_{2(g)} \rightarrow 2H_2O_{(g)}$$

Calculate the final volume of the container after the reaction is complete if the temperature remains constant.

Solution:

To calculate the final volume of the container after the reaction is complete, we can use the ideal gas law, assuming that the temperature remains constant.

Initial volume (V_1) = 5.00 L

Initial pressure (P_1) = 2.00 atm

T(K) = 27°C + 273.15 = 300.15 K

Initial moles of H_2 (n_1) = ?

The ideal gas law is given by: PV = nRT

We can find the initial moles of H_2 using the ideal gas law:

$$n_1 = (P_1V_1) / (RT_1)$$

$$2H_{2(g)} + O_{2(g)} \rightarrow 2H_2O_{(g)}$$

Since 2 moles of H_2 produce 2 moles of H_2O, the mole ratio is 1:1. This means that if all the H_2 reacts, the number of moles of H_2O produced will be the same as the initial moles of H_2. So, n_1 (initial moles of H_2) will also be the initial moles of H_2O formed.

Now, we can use the equation below to find the final volume (V_2) when the reaction is complete:

$$V_2 = (n_1RT_1) / P_1 = \frac{(n_1 \times 0.0821 L{\cdot}atm / (mol{\cdot}K) \times 300.15 K)}{2.00 atm} \approx 7.82 L$$

Therefore, the final volume of the container after the reaction is complete, assuming constant temperature, is approximately 7.82 L.

Applications in Real-World Chemistry:

Stoichiometry, a fundamental concept in chemistry, holds immense importance in various industries, including pharmaceuticals, agriculture, and environmental science. It serves as the quantitative foundation for optimizing processes, ensuring product quality, and addressing environmental concerns.

In the pharmaceutical industry, stoichiometry is indispensable for precise drug synthesis and formulation, guaranteeing the production of pharmaceutical compounds

with the desired purity and efficacy. In agriculture, stoichiometry aids in fertilizer production, determining the optimal nutrient ratios to promote plant growth while minimizing environmental impact. It also plays a crucial role in pesticide formulation, allowing for precise concentrations to control pests while safeguarding ecosystems.

Environmental science benefits from stoichiometry in pollutant monitoring and source identification, facilitating environmental impact assessments. It guides chemical dosing in wastewater treatment, ensuring efficient pollutant removal and reducing the generation of harmful byproducts. Stoichiometry is equally essential in the food industry, where it ensures accurate ingredient proportions and nutritional calculations to maintain product consistency. It also plays a vital role in brewing and fermentation processes, maintaining precise ratios for beverage and fermented food production.

Stoichiometric calculations inform various processes across different domains. In drug synthesis, they ensure precision and efficiency by minimizing waste and production costs. Stoichiometry aids in purity assessment by allowing chemists to compare actual yields to theoretical yields, guiding purification processes. In large-scale drug manufacturing, it ensures consistent product quality and reliability.

In the context of pollutant monitoring, stoichiometric calculations are indispensable for quantifying pollutant concentrations, facilitating regulatory compliance, and conducting environmental impact assessments. Furthermore, stoichiometry assists in source identification, as different pollutant sources release substances with distinct stoichiometric ratios, enabling accurate tracing of pollution origins. Stoichiometry significantly contributes to environmental impact assessments by revealing how pollutants disrupt natural systems, guiding conservation and remediation efforts. These diverse applications underscore the versatile and critical role of stoichiometry in various processes, from drug synthesis to environmental protection.

Conclusion

This chapter has revealed a comprehensive exploration of fundamental concepts in quantitative chemistry. Beginning with mole, conversion of gram into mole and molecules and the chemical equations their balancing by algebraic method, we ventured into the world of mole concepts and Avogadro's number, enabling us to seamlessly convert between mass and moles. The concept of the limiting reactant revealed how one key component can determine the extent of a reaction, while actual and theoretical yield calculations shed light on real-world complexities in chemical processes. We also delved into empirical and molecular formulas, essential tools for

deciphering compound compositions, and applied these concepts to practical scenarios. Gas stoichiometry expanded our horizons to encompass gas-phase reactions, while complex stoichiometry problems showcased the versatility of these principles in solving real-world chemical puzzles. Stoichiometry's versatility enhances efficiency and sustainability in these fields, driving advancements in healthcare, agriculture, and environmental protection.

Summary

Stoichiometry is the common language of chemistry, chemical engineering and chemical technology explaining its principles, applications, and significance in understanding chemical reactions and their quantitative relationships. Preliminary it is establishing a solid foundation, elucidating crucial concepts like atoms, molecules, and moles. Stoichiometry operates at the atomic level, highlighting the mole concept's role in bridging macroscopic and microscopic areas. To calculate the quantity of reactants and its respective product we need a balance chemical equation which is showcasing how it reflects mass and mole conservation. Herein we elaborate an algebraic way to balance a very complex reaction in a very simple mathematical way. The Practical examples are discussed, and the provision of step-by-step solutions enhances understanding. Stoichiometric coefficients' vital role in chemical equations is detailed, enabling the calculation of reactant consumption and product formation. The chapter explores limiting reactants, explaining their influence on reaction extent. Discussions on identifying limiting reactants and calculating percent yield enhance efficiency assessment. Stoichiometry extends beyond theory; its practical applications span environmental science, pharmacy, and industry, including pollution control, pharmaceutical formulation, and chemical manufacturing. Real world problems encompass reaction stoichiometry and stoichiometry of gases catering to those seeking deeper insights. Exercises and problems engage readers in applying stoichiometric knowledge, with detailed solutions provided for reinforcement. This chapter underscores stoichiometry's pivotal role as chemistry's language. It facilitates comprehension and control of chemical transformations, applicable in laboratories and industrial processes. This concise yet comprehensive chapter equips readers with essential knowledge and problem-solving skills, making stoichiometry an indispensable resource for students as well as teachers and other readers.

Scientific Ethics Declaration

The authors say that they are responsible for the scientific, moral, and legal aspects of this chapter, which is published in *Chemistry for the Life.*

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Conflict of Interest

The authors declare no conflict of interest.

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