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Unveiling Chemical Harmony through Diophantine Equations

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Abstract: Diophantine equations, characterized by algebraic polynomials with integer coefficients and multiple unknowns, are uniquely valuable for problems requiring integer solutions.

Their applicability spans diverse domains, including predicting economic trends, optimizing transportation costs, estimating profit margins, tailoring medication dosages to individual patient weights, resolving geometric dilemmas in physics, advancing cryptographic methodologies, addressing computational challenges, and refining chemical reaction equations. This paper delves into the innovative use of Diophantine equations as a mathematical framework for balancing chemical equations, accompanied by illustrative examples that showcase the method's practicality and precision. Also, the method of finding molecular formula of a chemical compound is also shown.

Keywords: Diophantine equations, Chemical Reaction, Molecular Formula, Balanced reaction, Unbalanced reaction.

I. INTRODUCTION

Number theory is a vast and intricate field within mathematics, deeply intertwined with numerous other mathematical disciplines. Often hailed as the purest form of mathematical study, it has traditionally been perceived as having limited direct applicability to real-world scenarios.

Nevertheless, its profound significance cannot be overstated, as it occupies a central role in the evolution of mathematical thought. Its fundamental principles, conjectures, and unresolved questions have been instrumental in shaping diverse mathematical frameworks and methodologies. From algebra and geometry to cryptography and computational sciences, its impact extends well beyond its initial theoretical boundaries, contributing substantially to both foundational research and practical innovations across multiple scientific domains.[1-5]

When atoms acquire or relinquish electrons, they transform into ions, or they may combine with other atoms to form molecules. This transformation necessitates a change or fusion of their symbols to generate an appropriate chemical formula that accurately represents the resulting species. Expanding this symbolic representation further allows for the depiction of both the identities and the relative quantities of substances involved in a chemical or physical transformation. This process is accomplished through the formulation and balancing of chemical equations. From a chemist's perspective, the most elementary and widely adopted approach for balancing chemical equations is either by direct inspection or by considering molecular weights. However, a mathematician approaches this task differently, treating chemical equations as algebraic expressions and solving them using systematic mathematical techniques. One such method involves the application of Diophantine equations, a branch of number theory that deals with integer solutions to polynomial equations.

A fundamental linear Diophantine equation takes the form $ax + by = c$, where a and b are integers, and x, y are variables representing unknown quantities. If a and b are relatively prime and the equation is expressed with $c = 1$, then an infinite number of solutions exist. Moreover, for any general case, a solution is guaranteed to exist if and only if the greatest common divisor (gcd) of a and b divides c. Conversely, if gcd(a, b) does not divide c, then the equation has no possible solutions[6-11]. This mathematical principle provides a structured and rigorous method for balancing chemical equations, demonstrating how number theory offers valuable insights into fundamental scientific processes. The author of [12] gives the application of Diophantine equation in solving chemical reaction.

This paper examines multiple chemical reactions, interpreting them through the framework of linear Diophantine equations and also finding Molecular formula for a substance. Each reaction is systematically analyzed and balanced using this mathematical approach to ensure accuracy and consistency in representation.

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II. METHODOLOGY

A. Balancing Chemical Reactions

This study examines multiple chemical equations that describe the formation of various chemical compounds and their corresponding byproducts. Each of these equations is systematically analyzed and balanced using the framework of linear Diophantine equations. By approaching chemical reactions from a mathematical perspective, we ensure precision in the representation of reactants and products while maintaining the integrity of mass and stoichiometric relationships. The balancing process follows the principles of Diophantine equations, where integer solutions govern the quantitative relationships between different substances involved in the reaction. This approach highlights the intrinsic connection between algebraic number theory and chemical transformations, demonstrating how mathematical techniques can be effectively employed to achieve accurate and consistent chemical equation balancing.

Consider,

$$\omega_1 \alpha_{\omega_1'} \beta_{\omega_2'} \gamma_{\omega_3'} + \omega_2 \alpha_{\omega_1''} \beta_{\omega_2''} \gamma_{\omega_3''} + \omega_3 \alpha_{\omega_1'''} \beta_{\omega_2'''} \gamma_{\omega_3'''} \rightarrow W_1 \alpha_{W_1'} \beta_{W_2'} \gamma_{W_3'} + W_2 \alpha_{W_1''} \beta_{W_2''} \gamma_{W_3''} + W_3 \alpha_{W_1'''} \beta_{W_2'''} \gamma_{W_3'''} \qquad (1)$$

This equations (1) yields the following system of equations:

$$\omega_1 \omega_1' + \omega_2 \omega_1'' + \omega_3 \omega_1''' = W_1 W_1' + W_2 W_1'' + W_3 W_1'''$$
$$\omega_1 \omega_2' + \omega_2 \omega_2'' + \omega_3 \omega_2''' = W_1 W_2' + W_2 W_2'' + W_3 W_2'''$$
$$\omega_1 \omega_3' + \omega_2 \omega_3'' + \omega_3 \omega_3''' = W_1 W_3' + W_2 W_3'' + W_3 W_3'''$$

Here α, β, γ are the chemical compound and $\omega_i', \omega_i'', \omega_i''', W_i', W_i'', W_i''' \in \mathbb{W}$, where $i = 1,2,3$. The coefficients $\omega_1, \omega_2, \omega_3, W_1, W_2, W_3$ serve as crucial numerical factors that dictate the proportional relationships between reactants and products within the given chemical equation. The above system of equation represents a fundamental Diophantine equation, offering a comprehensive set of integer solutions that maintain the integrity of stoichiometric balance. This equation ensures that the conservation of mass principle is upheld, providing a structured mathematical framework for accurately determining the quantitative interactions between various chemical species involved in the reaction.

B. Finding Molecular Forumula

Consider a substance with a molecular weight M, composed of two elements, X and Y, whose atomic weights are α and β, respectively. The molecular composition satisfies the equation:

$$\alpha\, u + \beta\, v = M \qquad \text{(A)}$$

where u and v are positive integers representing the number of atoms of X and Y within the molecule. For this expression to qualify as a Diophantine equation, the values of α, β and M must be integers.

If α and β are integers, then M will inherently be an integer. However, let I_α and I_β denote the nearest integer values of α and β. If the deviations $(\alpha - I_\alpha)$ and $(\beta - I_\beta)$ are sufficiently small, ensuring that:

$$-\frac{1}{2} < (\alpha - I_\alpha)u + (\beta - I_\beta)v < \frac{1}{2}$$

for reasonably small values of u and v typically found within a molecular structure, then the equation simplifies to:

$$I_\alpha u + I_\beta\, v = I_M \qquad \text{(B)}$$

where I_M is the integer closest to M. This refined equation takes the form of a Diophantine equation, which can be effectively solved to determine the integer values of u and v. In this way, a molecular formula for any substance involving 'n' chemical compounds can be found using linear Diophantine equation with 'n' unknowns.

III.RESULTS AND DISCUSSIONS

A. Few examples on Balancing Chemical Reaction

1) Illustration 1

Hydrolysis: The hydrolysis of sodium aluminate ($NaAlO_2$) in water leads to the formation of sodium hydroxide (NaOH) and aluminum hydroxide ($Al(OH)_3$). This reaction is widely utilized in industrial applications and water treatment processes. The related unbalanced chemical equation is given by

$$NaAlO_2 + H_2O \rightarrow NaOH + Al(OH)_3 \quad (2)$$

In order to balance the above chemical equation, consider

$$\omega_1 NaAlO_2 + \omega_2 H_2O \rightarrow W_1 NaOH + W_2 Al(OH)_3 \quad (3)$$

where $\omega_1, \omega_2, W_1, W_2 \in \mathbb{Z}$.

From the above equation (2), the following system of equation is formulated.

$$\omega_1 = W_1 \quad \text{(for } Na\text{)} \quad (4)$$

$$\omega_1 = W_2 \quad \text{(for Al)} \quad (5)$$

$$2\omega_2 = W_1 + 3W_2 \quad \text{(for H)} \quad (6)$$

$$2\omega_1 + \omega_2 = W_1 + 3W_2 \quad \text{(for O)} \quad (7)$$

From (4) and (5),

$$\omega_1 = W_1 = W_2$$

Using the above relation, (6) and (7) reduces to

$$2\omega_2 = 4\omega_1$$

$$\omega_2 = 2\omega_1$$

The above relation is linear equation in two variables which has a solution $[\omega_1, \omega_2] = [1,2]$. This may further leads to the solution of the system of linear Diophantine equations as $[\omega_1, \omega_2, W_1, W_2] = [1,2,1,1]$.

Hence the chemical equation (3) becomes,

$$NaAlO_2 + 2H_2O \rightarrow NaOH + Al(OH)_3,$$

which is balanced.

2) Illustration 2:

Reaction of Aluminium with Sodium Hydroxide : This reaction illustrates the interaction between aluminum (Al), sodium hydroxide (NaOH), and water (H_2O), resulting in the formation of sodium aluminate ($NaAlO_2$) and hydrogen gas (H_2). The corresponding unbalanced chemical equation is provided by

$$\omega_1 Al + \omega_2 NaOH + \omega_3 H_2O \rightarrow W_1 NaAlO_2 + W_2 H_2 \quad (8)$$

From the above equation (8), the following system of equation can be obtained

$$\omega_1 = W_1 \quad \text{for Al} \quad (9)$$

$$\omega_2 = W_1 \quad \text{for Na} \quad (10)$$

$$\omega_2 + \omega_3 = 2W_1 \quad \text{for O} \quad (11)$$

$$\omega_2 + 2\omega_3 = 2W_2 \quad \text{for H} \quad (12)$$

According to equation (9) and (10),

$$\omega_1 = \omega_2 = W_1 \quad (13)$$

With the help of (13), the equation (11) and (12) turns to

$3W_1 = 2W_2$

Thus, the above system has the solution $[\omega_1, \omega_2, \omega_3, W_1, W_2] = [2,2,2,2,3]$

Hence the balanced reaction is

$$2Al + 2NaOH + 2H_2O \rightarrow 2NaAlO_2 + 3H_2$$

3) Illustration 3

Combustion Chemical Reaction: A combustion reaction is a type of chemical process where a fuel reacts with an oxidizing agent, triggering its transformation and releasing energy, often in the form of heat and light. The unbalanced chemical reaction is given by

$\omega_1 CH_4 + \omega_2 O_2 \rightarrow W_1 CO_2 + W_2 H_2O$

The system of equation resulted from the above chemical reaction is:

$$\omega_1 = W_1 \quad \text{(for } C\text{)} \tag{14}$$

$$2\omega_2 = 2W_1 + W_2 \quad \text{(for O)} \tag{15}$$

$$4\omega_1 = 2W_2 \quad \text{(for H)} \tag{16}$$

From (14) and (16), the solution of $[\omega_1, \omega_2, W_1, W_2] = [1,2,1,2]$. Hence the balanced equation is shown as in the figure 1.

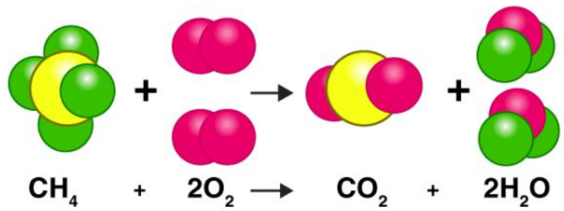

Fig 1: Combustion

B. Illustration of finding Molecular Formula using Diophantine equation

1) Illustration

Suppose a substance is composed of only Carbon and Hydrogen whose Molecular weight is 50.06 g/mol. In order to construct the molecular formula of the substance, consider the atomic mass of carbon and hydrogen.

Let u and v denotes the number of atoms of Carbon and Hydrogen respectively.

Atomic mass of Carbon = 12.011 g/mol

Atomic mass of Hydrogen = 1.008 g/mol

We have

$$12.011\ u + 1.008\ v = 50.01$$

Since $12.011 - 12 = 0.011$ and $1.008 - 1 = 0.008$ are so small. Thus,

$$12\ u + 1\ v = 50$$

The above equation has four possible positive integer solutions (u,v) namely $(1,38), (2,26), (3,14)$ and $(4,2)$. Among this $u = 4$ and $v = 2$ is the only positive integer solution which enhance the stability of the chemical compound. Hence the molecular formula is C_4H_2, commonly referred to as **Diacetylene** or **Butadiyne**, is an organic molecule characterized by two triple bonds, making it the simplest member of the polyyne family. With a molecular weight of **50.06 g/mol**, it exists as a colorless gas. This compound has been identified in **Titan's atmosphere** and in certain nebulae, where it forms through reactions involving acetylene. The structural arrangement of Diacetylene is given in the figure 2.

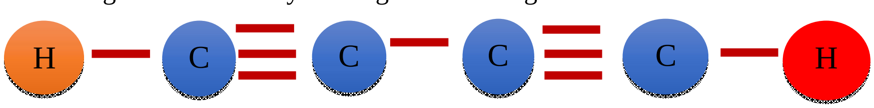

Fig 2: Chemical bond of Diacetylene

2) Illustration 2

Consider a compound consisting solely of carbon, hydrogen and Oxygen atoms with a molecular weight of 76.10 g/mol. To determine its molecular formula, take into account the atomic masses of carbon and hydrogen as below.

Let the number of atoms of Carbon, Hydrogen and Oxygen be u, v, w respectively

Atomic mass of Carbon = 12.011 g/mol

Atomic mass of Hydrogen = 1.008 g/mol

Atomic mass of Oxygen = 15.9994 g/mol

It is noted that

$$12.011\ u + 1.008\ v + 15.9994\ w = 76.10$$

Since the difference between 12.011, 1.008 and 15.9994 and the respective nearest integer value of 12.011, 1.008 and 15.9994 is so small, the following Diophantine equation is considered.

$$12u + v + 16w = 76$$

The possible positive integer solution for (u,v,w) are (1,48,1), (2,36,1) , (3,24,1), (4,12,1), (1,32,2), (2,20,2), (3,8,2), (1,16,3), (2,4,3). Among these solution, only guarentees the chemical stability of the substance.

Thus the molecular formula of the compound is $C_3H_8O_2$, which corresponds to **propylene glycol**, also known as **1,2-propanediol**. This compound is a clear, almost scentless liquid with a faintly sweet flavor, and it falls under the category of **diols**, which are characterized by having two hydroxyl **(–OH)** functional groups.

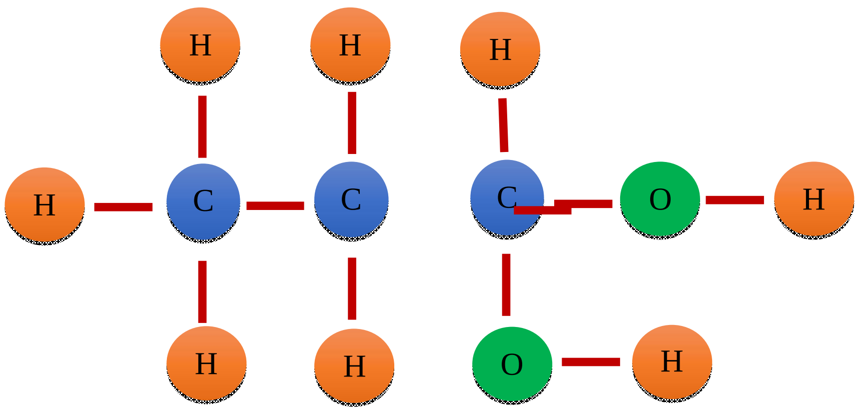

Fig 3: Chemical bond of propylene glycol

IV. CONCLUSIONS

Thus, the exploration of Diophantine equations as a tool for chemical analysis affirms their potency beyond traditional mathematical boundaries. By recasting chemical equation balancing and molecular formula determination into solvable systems of integer constraints, this approach exemplifies both analytical rigor and interdisciplinary versatility. The illustrative examples not only demonstrate the method's precision and scalability but also underscore its potential as a didactic resource and a computational asset in fields that demand exactitude. This fusion of number theory with chemical structure offers a promising avenue for future innovation at the intersection of mathematics and the natural sciences.

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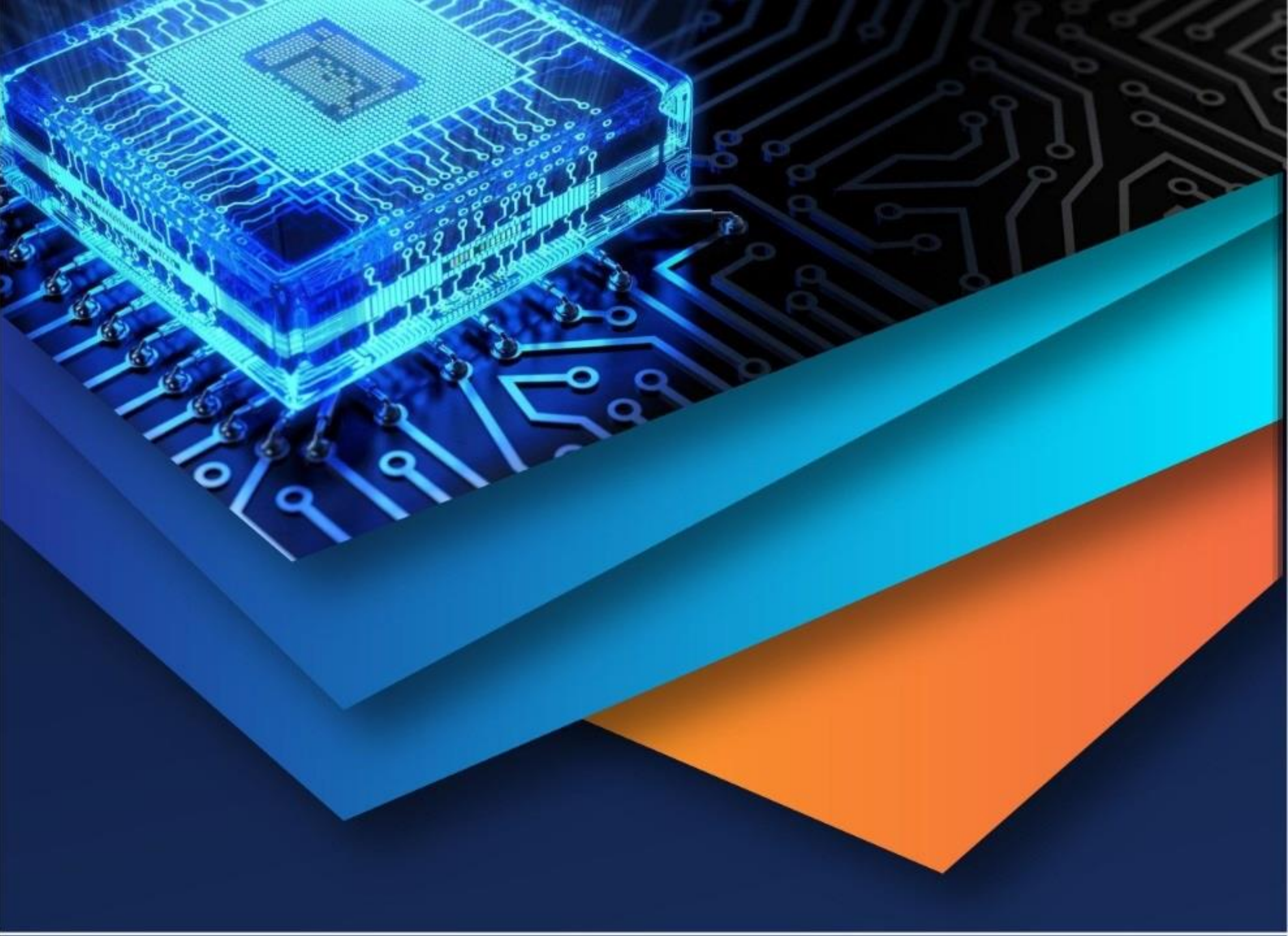

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