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An Innovative Method to Understanding Empirical and Molecular Formula of the Chemical Compounds in Numerical Problems

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ABSTRACT

In this study, we have used a simple and innovative theoretical method for identification of several carbon or other elements such as Nitrogen, oxygen, halogens etc., in the chemical numerical problems, generally, high school and undergraduate students face many difficulties during the solution of numerical problems regarding the empirical as well as the molecular formula of the chemical compounds. Identification and estimation of elements can be done by using the qualitative and quantitative analysis technique respectively, but to find out how many elements are there in the analytical sample to get difficulties, there are various methods are available but are time-consuming and students can't understand properly, so this new method is simple and innovative for getting the proper idea to easily understand and solving the numerical problems within the less time of the number of elements and easily calculate the empirical formula as well as the molecular formula of the chemical compounds.

Keywords: Empirical formula, Molecular formula, Qualitative analysis, quantitative analysis

INTRODUCTION

Analytical chemistry helps to identify the chemical composition i.e. chemical and physical data of analytical samples or substance. [2] In which also employed various innovative methods such as concentration terms, [6] redox titrations [3] etc., useful for identification and quantification of chemical composition. The key role of analysis as qualitative and quantitative. [1] The qualitative analysis provides the presence or absence of an element i.e. Identification and the relative proportion of an element and also estimation provides the quantitative analysis. [5] Determine the molecular formula of analytical compounds with the help of quantitative analysis molecular formula method of the compound indicator the actual number of an atom of the constituent elements in a molecule, it can be obtained from experimentally determined values of per cent element composition and molar mass of that compound quantitative determination of the constituent element by suitable methods provider the per cent elemental composition of a compound from the per cent composition, the ratio of the atom of the constituent elements in the molecule is calculated. [4]

THEORETICAL METHOD

The old method for determination of the molecular formula. In this method consist of six steps of determining the molecular formula of a compound in that they first find out empirical formula after that the molecular formula.

Step 1: check whether the sum of all percentage is 100 if the total per cent is not 100 then the difference is considered as per cent of oxygen.

Step 2: conversion of a mass per cent into grams.
Step 3: finding the moles of the atom.
Step 4: Divide the mole obtained above by the smallest value among them.
Step 5: Write the empirical formula by maintaining the number after writing the symbol of the respective element.
Step 6: Finally write the molecular formula.
(a). Determine empirical formula mass: Add the atomic masses of various atoms present in the empirical formula.
(b). Divide molar mass by empirical formula mass
= (molar mass) / (Empirical formula mass).
(c). multiply empirical formula by r obtain above to get the molecular formula.
Molecular formula = r x empirical formula.

New method: In our innovative method, used a simple and unique method to find out moles and empirical formula. We can directly find the number of atoms and the molecular formula.

By using the following formula's

Numbers of atom's

$$= \frac{\%\ of\ atom * Total\ mass\ of\ compound}{molarmass\ of\ atom * 100}$$

Examples 1:

A compound contains 4.07 % hydrogen, 24.27 % carbon and 71.65 % Chlorine by mass. Its molar mass is 98.96 g. What is its empirical formula? Atomic masses of hydrogen, carbon and chlorine are 1.008, 12.000 and 35.453 respectively.

Ans. (Old method):

Step 1: Check whether the sum of all the percentage is 100.

4.07 + 24.27 + 71.65 = 99.99 =100

Therefore, no need to consider the presence of an oxygen atom in the molecule.

Step 2: Conversion of a mass per cent into grams. Since we are having a mass present, it is convenient to use 100 g of the compound at the starting material. Thus, in the 100 g sample of the above compound, 4.07 g hydrogen 24.27 g carbon and 71.65 g chlorine are present.

Step 3: Convert grams into the number of moles of each element. Divide the masses obtained above by respective atomic masses of various elements.

Moles of hydrogen = $\frac{4.07\ g}{1.008\ g} = 4.04$

Moles of hydrogen = $\frac{24.27\ g}{12.01\ g} = 2.0225$

Moles of chlorine = $\frac{71.65\ g}{35.453\ g} = 2.021$

Step 4: Divide the mole value obtained above by the smallest value among them.

Since 2.021 is the smallest value, division by it gives ratio 2:1:1 for H:C: Cl.

In case the ratio are not whole numbers, then they may be converted into the whole number by multiplying by the suitable coefficient

Step 5: writing the molecular formula

Determine empirical formula mass: Add the atomic masses of various atoms present in the empirical formula. For CH_2Cl, empirical formula mass is 12.01 + 2 x 1.008 + 34.453 = 49.48 g

Divide mass by the empirical formula is:

$\frac{molar\ mass}{Emprical\ formula\ mass} = \frac{98.96\ g}{49.48\ g}$,

r = 2

Multiple empirical formulae by r obtained above to get the molecular formula.

Molecular formula = r x empirical formula

Molecular formula is 2 x CH_2Cl i.e. $C_2H_4Cl_2$.

(New method)

% of H = 4.07, % of C = 24.27, % of Cl = 71.65.

The total mass of compound 98.96.

Numbers of a carbon atom

$$= \frac{\%\ of\ \ carbon\ atom * Total\ mass\ of\ compound}{molar\ mass\ \ carbon\ of\ atom * 100}$$

$= \frac{24.27 * 98.96}{12 * 100}$, X = 2

Number of carbons is 2.

No. of the hydrogen atom

$$= \frac{\%\ of\ hydrogen\ atom * total\ mass\ of\ compound}{molar\ mass\ of\ hydrogen\ atom * 100}$$

$= \frac{4.07 * 98.96}{1 * 100}$

No. of hydrogen atom = 4.02

Numbers of Cl atom's

$$= \frac{\%\ of\ \ Cl\ \ atom * Total\ mass\ of\ compound}{molar\ \ mass\ cl\ of\ atom * 100}$$

$= \frac{71.65 * 98.96}{35.5 * 100}$ = 7064.69/3550 = 1.9900.

Number if Cl is 2.

Then C = 2, H = 4, Cl = 2.

Molecular formula = $C_2H_4Cl_2$.

Example 2:

A compound with molar mass 159 was found to contain 39.62% copper and 20.13% sulfur suggest a molecular formula for the compound.

Ans (new method):

% of copper = 39.62 %, % of Sulphur = 20.13 %

% of oxygen = 40.25 %

No. of Cu atoms

$$= \frac{\%\ of\ cupper\ atom * Total\ mass\ of compound}{mass\ of\ cupper * 100}$$

$$= \frac{39.62 * 159}{63 * 100}$$

No. of copper Atom = 0.99999 ~ 1

No. of S atom

$$= \frac{\%\ of\ sulphur\ \ atom * Total\ mass\ of compound}{mass\ of\ sulphur\ * 100}$$

$$= \frac{20.13 * 159}{32 * 100}$$

No. of S Atom = 1, No. of Oxygen Atom

$$= \frac{\%\ of\ \ Oxygen\ \ atom * Total\ mass\ of compound}{Mass\ of\ oxygen\ atom * 100}$$

$= \frac{40.25 * 159}{16 * 100} = 3.9998 \sim 4$

No. of 'O' Atom = 4

Then Molecular formula = $CuSO_4$

Example 3:

Ans: % of carbon = 20 %, % of hydrogen = 6.7 %

% of nitrogen = 46.67 %, Total mass = 60

Numbers of carbon atoms

$$= \frac{\%\ of carbon\ \ atom * Total\ mass\ of\ compound}{molar mass\ of carbon\ \ atom * 100} = \frac{20 * 60}{12 * 100}$$

No. of carbon atom = 1

Numbers of H atom's

$$= \frac{\%\ of H\ \ atom * Total\ mass\ of\ compound}{molar\ mass\ of\ H\ atom * 100} = \frac{6.7 * 60}{1 * 100}$$

= 4.02

Numbers of Nitrogen atom's

$$= \frac{\%\ of\ N\ atom * Total\ mass\ of\ compound}{molar\ mass\ of\ Natom * 100} = \frac{46.67 * 60}{14 * 100}$$

No. of Nitrogen atom = 2

Numbers of oxygen atoms

$$= \frac{\%\ of\ O\ atom * Total\ mass\ of\ compound}{molar\ mass\ of\ \ O\ atom * 100} = \frac{26.63 * 60}{16 * 100}$$

= 0.9998 ~ 1

No. of oxygen atom = 1, Chemical formula CH_4N_2O

CONCLUSION

In this study, we have provided the innovative numerical method for investigation of several elements such as carbon, nitrogen, oxygen, halogens, etc., there are various methods are employed but students face difficulties, therefore this simple and unique method is suitable. High school and undergraduate students can be easily understood and solve such types of chemical numerical problems.

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