The Empirical Formula and The Molecular Formula

The empirical formula is the simplest formula that exists in simplest whole numbered ratios. That is, it gives the number of moles of each element present in the lowest possible numbers. If you know the number of moles of each element, then you can write the empirical formula. Let us say that 2 moles of A combines with 3 moles of B, then the empirical formula becomes A_2B_3. If 7 moles of A combines with 5 moles of B and 11 moles C, then the empirical formula becomes $A_7B_5C_{11}$.

Suppose a sample of water is decomposed in the laboratory and found that it produced 0.510 g of hydrogen and 4.08 g of oxygen. In order to calculate the empirical formula, firstly grams have to be converted into moles (divide the mass by molar mass) , secondly the mole ratio is calculated, and thirdly the empirical formula is written. These steps are summarized below.

mass(g) → **moles** → **mole ratio** → **empirical formula**
step 1 step 2 step 3

Step 1:

mol H = 0.510 g/ 1.008 g/mol = 0.506 mol H
mol O = 4.08 g / 16.0 g/mol = 0.255 mol O

These data indicates that there are 0.506 mol H for every 0.255 mol O. Based on this, the empirical formula assumes,

$$H_{0.50595}\,O_{0.255}$$

However, these fractions have to be converted into integer whole numbers that is done in the next step.

Step 2:

To take the mole ratio, divide each mole by the smallest mole. Between the moles of H and O, the smallest mole is 0.255. Divide 0.506 by 0.255 and 0.255 by 0.255 to get the mole ratio. If possible, round the resulting mole to a nearest integer.

mol H = 0.506 mol / 0.255 = 1.98 mol = 2 mol
mol O = 0.255 mol / 0.255 = 1 mol

Step 3:

Now write the final empirical formula based on the mole ratio, which is,

H_2O

Example

In the laboratory, an experiment is carried to decompose a compound containing nitrogen and oxygen and found that 8.167 grams of nitrogen and 23.33 grams of oxygen are produced. Determine the empirical formula of the compound.

Answer

Step 1: To get the moles, divide the masses by their corresponding molar masses.

mol N = 8.167 g / 14.01 g/mol = 0.583 mol N
mol O = 23.33 / 16.0 g/mol = 1.458 mol O

Step 2: Divide each mol with 0.583 to get the mol ratio.

mol N = 0.583 mol / 0.583 = 1 mol N
mol O = 1.458 mol / 0.583 = 2.5 mol O

Step 3: Write the empirical formula, which is

$N\,O_{2.5}$

But the number of moles of O is not a whole number. To convert that fraction into a whole number, multiply the moles of N and moles of O with 2. That is,

$2 \text{ x } N\,O_{2.5} = \quad N_2O_5$

Therefore the proper empirical formula is N_2O_5.

Example

A student burned the magnesium in a crucible and found that the residue contains 72.93 % magnesium 28.02 % oxygen. Calculate the empirical formula.

Answer

The problem is stated in terms of percents. However, we need mass (g) to get the moles. Therefore, we need to convert the percents into mass (g). The easiest way is to assume 100 g of sample. Then the percents automatically become grams, that is,

72.93 % Mg = 72.93 g Mg and 28.02 % O = 28.02 g O

Then exactly the same procedure as outlined in the previous problem is followed to deduce the empirical formula.

Step 1: Divide the mass by the molar mass to get the moles.

mol Mg = 72.93 g / 24.31 g/mol = 3 mol Mg
mol O = 28.02 g / 14.01 g/mol = 2 mol NO

Step 2: The moles obtained in step 2 are already in smallest whole numbers. Hence, the correct empirical formula is

Mg_2N_2

Molecular Formula

The formula deduced from percent composition or experimental masses always gives the empirical formula simply because the subscripts (moles of atoms) in the formula are in smallest whole numbers. In order to come with the actual molecular formula, the molar mass of the compound is needed that is usually obtained by some other methods.

The molar mass of the compound is always the integral multiple of the empirical formula mass. Consider for example H_2O_2, which has the empirical formula HO. The molar mass of HO is 17 g and that of H_2O_2 is 34 g. The molar mass (34 g) is twice the molar empirical formula mass (17 g). In general,

Molar mass = n x Molar empirical formula mass, n =1, 2, 3, …

The above statement in terms formulas becomes,

Molecular formula = n x Empirical formula, = 1, 2, 3, …, n

Let us illustrate this concept with the following example.

Example

A sample of compound containing carbon (C) and hydrogen (H) has been analyzed and found that it contains 10.51 g of C and 1.75 g of H. The molar mass of the compound determined from other experiment is about 28 g. What is the molecular formula of the compound?

Answer

First the empirical formula has to be deduced and then the molecular formula. To obtain the empirical formula, apply the procedure described in the previous examples.

mol C = 10.51 g / 12.00 g/mol = 0.876 mol/0.876 = 1 mol
mol H = 1.75 g / 1 g /mol = 1.75 mol = 0.876 = 1.99 mol = 2 mol

Therefore, the empirical formula is CH_2. The molar mass of empirical formula is 14g (12 g + 2 g). The given molar mass (28 g) is twice the molar empirical formula mass. Hence,

Molecular formula = 2 x CH_2 = C_2H_4
