Empirical Formula & Molecular Formula

Initially, chemical formulas were obtained by determination of masses of all the elements that are combined to form a molecule and subsequently we come up with two important types of formulas in chemistry : *molecular formula and empirical formula*.

The empirical formula of a compound gives the simplest ratio of the number of different atoms present, whereas the molecular formula gives the actual number of each different atom present in a molecule. If the formula is simplified then it is an empirical formula. The molecular formula is commonly used and is a multiple of the empirical formula.

The general statement relating molecular formula and the empirical formula is

Molecular Formula = n x Empirical Formula

What is Molecular formula?

- The molecular formula is the formula derived from molecules and is representative of the total number of individual atoms present in a molecule of a compound.
- A molecular formula uses a subscript that reports the actual number of each type of atom in a molecule of the compound.
- Molecular formulas are associated with gram molecular masses that are simple whole number multiples of the corresponding empirical formula mass.

What is Empirical formula?

- The empirical formula is the simplest formula for a compound which is defined as the ratio of subscripts of the smallest possible whole number of the elements present in the formula. It is also known as the simplest formula.

- An empirical formula for a compound is the formula of a substance written with the smallest integer subscript.
- The empirical formula gives information about the ratio of numbers of atoms in the compound. The percent composition of a compound directly leads to its empirical formula. Empirical Formula Vs Molecular Formula.

Empirical Formula	Molecular Formula
An empirical formula represents the simplest whole-number ratio of various atoms present in a compound	The molecular formula shows the exact number of different types of atoms present in a molecule of a compound.
Example : The empirical formula for Acetylene is CH .	Example : The molecular formula for Acetylene is C_2H_2 .

Example : Glucose Molecular Formula Vs Glucose Empirical Formula

Let's take the example of glucose. The molecular formula of glucose is $C_6H_{12}O_6$ and the empirical formula of glucose is CH_2O. We can derive a relation between the Molecular formula and the empirical formula of glucose.

Empirical Formula & Molecular Formula of Butane & Octane
[/caption]

$$C_6H_{12}O_6 = 6 \times CH_2O$$

We can derive a general expression as,

Molecular formula = n x empirical formula ; Where, ‘n’ is a whole number. Sometimes, the empirical formula and molecular formula both can be the same.

Question-1 : The empirical formula of Boron Hydride is BH3. Calculate the molecular formula when the measured mass of the compound is 27.66.

Solution :

The atomic mass is given by = B + 3(H) = 10.81 + 3(1) = 13.81 u
But, the measured molecular mass for Boron atom is given as 27.66 u. By using the expression,
Molecular formula = n x empirical formula n
= molecular formula/empirical formula
= 27.66 / 13.81
= 2
Putting the value of n = 2 in the empirical formula we get molecular formula as Molecular formula = $2(BH_3) = B_2H_6$.

Question-2 : The empirical formula of a compound is $COCl_2$ and its molecular mass is 90.00u. Find out the molecular formula of that compound.

Solution :

COCl2 = C + O + 2(Cl) = 12 + 16 + 2(35.5) = 99u
Empirical formula is the same as molecular mass as n=1, this means molecular formula is $COCl_2$.

Question-3 : What is the molecular formula of a compound which has an empirical formula of CH_2 and a relative molecular mass of 70?

Solution :

Relative molecular mass = 70
Empirical formula mass = 12 + 2 = 14

The relative molecular mass is 5 x the relative empirical formula mass
The molecular formula is 5 x the empirical formula The molecular formula is C_5H_{10} .

Question-4 : A compound of iron and oxygen is analysed and found to contain 69.94% iron and 30.06% oxygen. Find the empirical formula of the compound.

Solution :

Steps for Problem Solving	**Find the empirical formula of a compound of 69.94% iron and 30.06% oxygen.**
Identify the "Given information and what the problem is asking you to find."	Given : % of Fe = 69.94% % of O = 30.06% Find : Empirical Formula = $Fe_?O_?$
Calculate	
a. Assume a 100g sample, convert the same % value to grams.	69.94g Fe 30.06g O

b. Covert to moles.	69.94g Fe x $\frac{1\ mol\ Fe}{55.85g\ Fe}$ = 1.252 mol Fe 30.06g O x $\frac{1\ mol\ O}{16.00g\ O}$ = 1.879 mol O
c. Divide both moles by the smallest of the results.	Fe x $\frac{1\ .252\ mol}{1.252}$ O x $\frac{1.879\ mol}{1.252}$ The "non-whole" empirical formula of the compound is $Fe_1O_{1.5}$
d. Multiply each of the moles by the smallest whole number that will convert each into a whole number.	Since the moles of O is still not a whole number, both moles can be multiplied by 2, while rounding to a whole number.
e. Write the empirical formula	The empirical of the compound is Fe_2O_3