Determination of Empirical and Molecular Formula

- The simple formula that gives the simplest whole number ratio between the atoms of the various elements present in the compound is called its empirical formula.
- Empirical and molecular formulae of a compound can be determined from the composition of the compound, which is expressed in terms of the percentage of each element present in it.

1

Determination of Empirical Formula

- **Step 1**
  - Determine the percentage of each element present in the compound from the mass of each element present in a certain known mass of the compound.

2

Determination of Empirical Formula

- **Step 2**
  - If the sum of the percentages of all these elements is not 100, then the difference gives the percentage of oxygen. The percentage of oxygen in the given compound is calculated by using the following relationship.

    Percentage of oxygen = 100 - (sum of the percentages of all other elements)

3

Determination of Empirical Formula

- **Step 3**
  - The percentage of each element is divided by the atomic mass of the respective element.
  - The ratio so obtained is called 'atomic ratio'.

4

Determination of Empirical Formula

- **Step 4**
  - The atomic ratios is divided by the lowest value, and converted into the nearest whole numbers.
  - These whole numbers give the simplest ratio between the number of atoms of the various elements present in the compound.
  - This is the empirical formula.

5

Determination of Molecular Formula

- The molecular formula is then obtained by
- Molecular formula = n x Empirical formula

where, n is a whole number such as 1, 2 etc.

6

Exercises

- Determine the molecular formula for each compound below from the information listed.

substance	Simplest formula	Mol mass (g/mol)
Octane	C_4H_9	114
Ethanol	C_2H_6O	46
Naphthalene	C_5H_4	128
Glucose	CH_2O	180
Melamine	CH_2N_2	126

7

Example

- An organic compound weighing 0.2 g containing 40% C, 6.66 % H and O gave on combustion 0.296 g CO_2 and 0.12 g H_2O. Its molecular mass is 180. Determine its empirical and molecular formulae.

8

Solution

Weight of the compound taken = 0.2 g

Molar Mass of CO_2 formed = 0.296 g

Molar Mass of H_2O formed = 0.12 g

Therefore, the percentage of Oxygen

= 100 - (40.0 + 6.67)

= 53.33% (by difference)

9

Solution…

- Atomic mass of O =16, C=12, H=1
- Divide the respective percentages by the atomic masses of the elements.
  - i.e. for C: 40/12 = 3.33
  - For H: 6.66/1 = 6.66
  - For O: 53.33/16 = 3.33
- Divide the ratio by the lowest i.e.
  - 3.33/3.33 gives C=1
  - 6.66/3.33 gives H=2
  - 3.33/3.33 gives O =1
- Therefore, empirical formula of the compound = CH_2O

10

Solution…

- Mass for CH_2O is 12+(2 X 1)+16 = 30
- Molecular formula = n X empirical formula
- Its molecular mass is 180.
- 180 = n X 30, therefore n=6
- Molecular formula = 6 X (CH_2O) =$C_6H_{12}O_6$

11

Try to solve the following…

Calculate the molecular formula for the following

a. empirical formula CH, molar mass = 78 g/mol

b. empirical formula NO_2, molar mass = 92.02 g/mol

c. caffeine, 49.5% C, 5.15% H, 28.9% N, 16.5% O by mass, molar mass = 195 g.

12

Answers:

a. C_6H_6
b. N_2O_4
c. $C_8H_{10}N_4O_2$

More calculations

- Molecular formula can be used to determine the weights of various components of a complete combustion.

For example:

- 5.8g of butane is subjected complete combustion in oxygen. Determine the mass of:
  a) Oxygen required
  b) CO_2 and H_2O produced
  (Note: C=12, H=1, O=16)

Solution

- The molar mass of butane , C_4H_{10}, is:
- Relative Molar mass (RMM)= (4 × 12)+(10 × 1)
  = 58 g mol^{-1}
- Hence, the number of moles in 5.8 g of butane is:
- Moles = weight/RMM
  = 5.8g/58gmol-1
  = 0.10 moles

Solution…

- Now, the balanced equation for the complete combustion is:

  $2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O$

OR

  $C_4H_{10} + 13/2\ O_2 \rightarrow 4CO_2 + 5H_2O$

- In other words, 1 mole of butane reacts with 6.5 moles of oxygen to give 4 moles of Carbon dioxide and 5 moles of water.

Solution …

- Therefore 0.1 mole of butane reacts with 0.65 moles of oxygen to give 0.4 moles of CO_2 and 0.5 moles of H_2O.
- Using the relationship: weight = moles × RMM, it is easy to calculate the weight of oxygen, CO_2 and H_2O.
- Now:

  RMM of O_2 = 16 × 2 = 32

  RMM of CO_2 = 12+(2 × 16)= 44

  RMM of H_2O = (2 × 1)+16 =18

Solution…

Compound	RMM	moles	Weight (g) = RMM × moles
O_2	32	0.65	20.8
CO_2	44	0.4	17.6
H_2O	18	0.5	9.0