2.8 Calculation of empirical and molecular formula from % composition

Learning outcomes

After the completion of the chapter, the students should be able to:

- Find the empirical and molecular formula from the percentage composition.

Core Concepts

- **Empirical Formula:** The simplest whole-number ratio of atoms of each element present in a compound.
- **Molecular Formula:** The actual number of atoms of each element present in one molecule of the compound.
- **Relationship:** Molecular Formula = n × (Empirical Formula)

Where n = Molecular Weight / Empirical Formula Weight

- **Vapour Density Relationship:** For volatile organic compounds, the molecular weight can be determined via its Vapour Density (VD):

Molecular Weight = 2 × Vapour Density

Worked Examples (Formulas from % Composition)

Example 1: Investigation of a Plant Extract from Khaptad

Question: A plant sample was collected from the pristine alpine regions of Khaptad, Far-Western Nepal. Solvent extraction of the plant contents revealed the presence of a suspected organic acid. Elemental analysis showed that the compound consists of 40% Carbon, 6.66% Hydrogen, and 53.44% Oxygen. Nitrogen, sulphur, and halogens were absent. If the molecular weight of this acid is determined to be 60, calculate its empirical and molecular formulas.

Solution:

Step 1: Determine the Empirical Formula using an Element Ratio Table

Element	% by Mass	Atomic Mass	Relative Moles	Simple Ratio	Simplest Whole Ratio
Carbon (C)	40.00%	12	40.00 / 12 = 3.33	3.33 / 3.33 = 1	1
Hydrogen (H)	6.66%	1	6.66 / 1 = 6.66	6.66 / 3.33 = 2	2
Oxygen (O)	53.44%	16	53.44 / 16 = 3.34	3.34 / 3.33 = 1.003 ~ 1	1

Empirical Formula = **CH_2O**

Step 2: Determine the Molecular Formula

1. Empirical Formula Weight = 12 + (2 × 1) + 16 = 30 amu
2. Given Molecular Weight = 60
3. Find n: n = Molecular Weight / Empirical Formula Weight = 60 / 30 = 2
4. *Molecular Formula = 2 × (CH_2O) =* **$C_2H_4O_2$** (Acetic Acid / Ethanoic Acid)

Example 2: Organic Compound via Vapour Density

Question: An organic compound containing carbon, hydrogen, and oxygen gives the following mass composition: C = 40.687%, H = 5.085%, and O = 54.228%. The vapour density of the compound is measured to be 59. Calculate its empirical and molecular formulas.

Solution:

Step 1: Determine the Empirical Formula

Element	% by Mass	Atomic Mass	Relative Moles	Ratio	Simplest Whole Ratio
C	40.687%	12	40.687 / 12 = 3.390	3.390 / 3.389 = 1	2 (1 × 2)
H	5.085%	1	5.085 / 1 = 5.085	5.085 / 3.389 = 1.5	3 (1.5 × 2)
O	54.228%	16	54.228 / 16 = 3.389	3.389 / 3.389 = 1	2 (1 × 2)

Note: Because the structural ratio for H is 1.5, we multiply all numbers by 2 to achieve integers.

Empirical Formula = **$C_2H_3O_2$**

Step 2: Determine the Molecular Formula

1. Molecular Weight = 2 × Vapour Density = 2 × 59 = 118 g/mol
2. Empirical Formula Weight = (12 × 2) + (1 × 3) + (16 × 2) = 24 + 3 + 32 = 59 amu
3. Find n: n = 118 / 59 = 2
4. *Molecular Formula = 2 × ($C_2H_3O_2$) =* **$C_4H_6O_4$**

1. Write the relationship between the empirical formula and molecular formula of a compound. 1
2. A plant was collected from Khaptad, far western Nepal. From the solvent extraction of the plant contents, an acid was suspected. From elemental analysis, the compound was found to consist of 40% carbon, 6.66% hydrogen and 53.44% oxygen. Element detection shows the absence of nitrogen, sulphur, and halogens. The molecular weight of the acid was found to be 60. Determine the empirical formula and molecular formula of the acid.
3. An organic compound containing carbon, hydrogen and oxygen gave the following composition: C= 40.687%, H= 5.085% and O= 54.228%. The vapour density of the compound is 59. Calculate the empirical formula and molecular formula of the compound. 3
4. *Glucose contains 40 % C, 6.67% H and 53.3% O by mass. Calculate its empirical formula.* *3*

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