

DETERMINATION OF THE STRUCTURAL FORMULA OF AN UNKNOWN ORGANIC COMPOUND

The structural formula of an unknown organic compound can be determined in the following way:

- i) the qualitative composition is determined experimentally (i.e. the functional groups present are identified)
- ii) the quantitative composition is determined experimentally
- iii) the empirical formula is calculated from the quantitative composition
- iv) the relative molecular mass is determined experimentally
- v) the molecular formula is determined from the empirical formula and the molecular mass
- vi) using data from i) and v), a possible structural formula can be determined

Example

A compound of C, H, and O is burned in excess oxygen.

- a) If 1.243 g of the compound produces 2.48 g of carbon dioxide, and 1.01 g of water, find the empirical formula
- b) If 0.524 g of the compound occupies 0.148 L in the gaseous state at 20°C and 98.6 kPa, find the molecular formula.
- c) The compound dissolves in NaHCO₃ solution evolving CO₂. Suggest possible structural formulae.
- d) If the compound had not dissolved in NaHCO₃, what would be the possible structural formulae?

Answer:

- a) Calculation of the empirical formula:

$$\text{moles of CO}_2 = \frac{2.48}{44} = 0.05635 = \text{moles of C present}$$

$$\text{moles of H}_2\text{O} = \frac{1.01}{18} = 0.05606 \quad \text{i.e. moles of H present} = 2 \times 0.05606 = 0.1121$$

$$\text{mass of C present} = 0.05635 \times 12.01 = 0.6768 \text{ g}$$

$$\text{mass of H present} = 0.1121 \times 1.008 = 0.1130 \text{ g}$$

$$\text{i.e. mass of O present} = 1.243 - (0.6768 + 0.1130) = 0.4532 \text{ g}$$

$$\text{moles of O present} = \frac{0.4532}{16} = 0.02832$$

moles of	C	H	O
	0.05635	0.1121	0.02832
=			
=	1.99	3.96	1
\approx	2	4	1

i.e. empirical formula is $\text{C}_2\text{H}_4\text{O}$

b) Calculation of the molecular formula

$$PV = nRT \quad n = \frac{PV}{RT} = \frac{1.013 \times 10^5 \times 0.002}{8.314 \times 300} = 0.005990 \text{ moles}$$

$$\text{molar mass} = \frac{\text{mass}}{\text{moles}} = \frac{0.5175}{0.005990} = 87.5 \text{ g mol}^{-1}$$

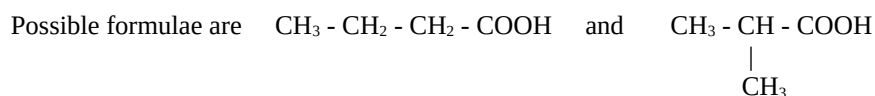
$$\text{molecular formula} = (\text{empirical formula}) \times n = (\text{C}_2\text{H}_4\text{O}) \times n$$

$$\text{i.e. } 87.5 = (24 + 4 + 16) \times n = 44 \times n$$

$$n = \frac{87.5}{44} \approx 2$$

Thus, the molecular formula is $(\text{C}_2\text{H}_4\text{O})_2$ or $\text{C}_4\text{H}_8\text{O}_2$

c) Acids react with hydrogencarbonates to form carbon dioxide, so the compound must be a carboxylic acid i.e. it must contain a $-\text{COOH}$ group.



d) If the compound had not reacted with NaHCO_3 , and yet it contains two oxygen atoms, then it must be an ester i.e. contain the group $-\text{COO}-$

