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 20oC and 98.6 kPa, find the molecular formula.

c) The compound dissolves in $NaHCO_3$ solution evolving CO_2. Suggest possible structural formulae.

d) If the compound had not dissolved in $NaHCO_3$, what would be the possible structural formulae?

Answer:

a) Calculation of the empirical formula:

moles of CO2 = = 0.05635 = moles of C present

moles of H_2O = = 0.05606 i.e. moles of H present = 2 x 0.05606 = 0.1121

mass of C present = 0.05635 x 12.01 = 0.6768 g

mass of H present = 0.1121 x 1.008 = 0.1130 g

i.e. mass of O present = 1.243 - (0.6768 + 0.1130) = 0.4532 g

moles of O present = = 0.02832

	C	H	O
moles of	0.05635	0.1121	0.02832
=			
=	1.99	3.96	1
≈	2	: 4	: 1

i.e. empirical formula is C_2H_4O

b) Calculation of the molecular formula

PV = nRT n = = = 0.005990 moles

molar mass = = = 87.5 g mol^{-1}

molecular formula = (empirical formula) x n = (C_2H_4O) x n

i.e. 87.5 = (24 + 4 + 16) x n = 44 x n

n = ≈ 2

Thus, the <u>molecular formula</u> is $(C_2H_4O)_2$ or $C_4H_8O_2$

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

Possible formulae are $CH_3 - CH_2 - CH_2 - COOH$ and $CH_3 - CH(CH_3) - COOH$

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 - COO -

Possible formulae are $CH_3 - CH_2 - C(=O) - O - CH_3$ $CH_3 - C(=O) - O - CH_2 - CH_3$

$H - C(=O) - O - CH_2 - CH_2 - CH_3$ $H - C(=O) - O - CH(CH_3) - CH_3$