**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 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:

 moles of CO2 = = 0.05635 = moles of C present

 moles of H2O = = 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

 moles of C H O

 0.05635 0.1121 0.02832

 =

 = 1.99 3.96 1

 ≈ 2 : 4 : 1

 i.e. empirical formula is C2H4O

 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 = (C2H4O) x n

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

 n = ≈ 2

 Thus, the molecular formula is (C2H4O)2 or C4H8O2

 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 CH3 - CH2 - CH2 - COOH and CH3 - CH - COOH

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 CH3

 d) If the compound had not reacted with NaHCO3, and yet it contains two oxygen atoms, then it must be an ester i.e. contain the group - COO -

 Possible formulae are CH3 - CH2 - C - O - CH3 CH3 - C - O - CH2 - CH3

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 O O

 H - C - O - CH2 - CH2 - CH3 H - C - O - CH - CH3

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 O O CH3