

Combustion Analysis

1. Cumene is a organic compound contains only carbon and hydrogen that is used in the production of acetone and phenol in the chemical industry. Combustion of 47.6 mg of cumene produces 156.8 mg of carbon dioxide and 42.8 mg of water. The molar mass of cumene is between 115 and 125 g/mole. Determine the molecular formula.
2. A combustion device was used to determine the empirical formula of an organic compound. A 0.6349 g sample was burned and produced 1.603 g of carbon dioxide and 0.2810 g of water and no other oxides. Determine the empirical formula for the compound.
3. The combustion analysis of 19.8mg of an organic acid produced 39.6 mg of carbon dioxide and 16.2 mg of water. The molar mass is ~88 g/mole. Determine the molecular formula.
4. A confiscated white substance, suspected of being cocaine, was purified by a forensic chemist and subjected to elemental analysis. Combustion of a 32.00 mg sample yielded 78.99 mg of carbon dioxide and 19.96 mg of water. Analysis for nitrogen showed that the compound contained 4.62 % N by mass. Calculate the empirical formula.

ANSWERS more on back....

1. Cumene is a organic compound contains only carbon and hydrogen that is used in the production of acetone and phenol in the chemical industry. Combustion of 47.6 mg of cumene produces 156.8 mg of carbon dioxide and 42.8 mg of water. The molar mass of cumene is between 115 and 125 g/mole. Determine the molecular formula.

In this problem you are told that the compound only contains carbon and hydrogen, so we can determine the number of moles of C and H immediately.

$$156.8\text{mgCO}_2 \left(\frac{1\text{mol}}{44\text{g}} \right) \left(\frac{1\text{C}}{1\text{CO}_2} \right) = 3.56\text{mmolC} \quad \frac{3.56\text{mmolC}}{3.56} = 1 \times 3 = 3\text{C}$$

$$42.8\text{mgH}_2\text{O} \left(\frac{1\text{mol}}{18\text{g}} \right) \left(\frac{2\text{H}}{1\text{H}_2\text{O}} \right) = 4.76\text{mmolH} \quad \frac{4.76\text{mmolH}}{3.56} = 1.33 \times 3 = 4\text{H}$$

thus the empirical formula is C_3H_4

To determine the molecular formula, you must calculate the molar mass of the empirical formula: $\text{C}_3\text{H}_4 = 40 \frac{\text{g}}{\text{mol}}$

Then divide the molar mass of the compound (I used the middle of the two values given) by the molar mass of the empirical formula: $\frac{120\text{g}}{40\text{mol}} = 3$ then "drive" this factor, through the empirical formula to give, C_9H_{12}

2. A combustion device was used to determine the empirical formula of an organic compound. A 0.6349 g sample was burned and produced 1.603 g of carbon dioxide and 0.2810 g of water and no other oxides. Determine the empirical formula for the compound.

In this problem you are only told that the compound is an organic compound, thus it will contain carbon and hydrogen, but it may also contain oxygen, and you need to check for that, by looking for any "missing mass."

$$0.2810\text{gH}_2\text{O}\left(\frac{2\text{g}}{18\text{g}}\right) = 0.0312\text{gH} \quad 1.603\text{gCO}_2\left(\frac{12\text{g}}{44\text{g}}\right) = 0.437\text{gC} \quad 0.6349\text{gTotal} - 0.437\text{gC} - 0.0312\text{gH} = 0.167\text{gO}$$

$$0.437\text{gC}\left(\frac{1\text{mol}}{12\text{g}}\right) = 0.0364\text{molC} \quad \frac{0.0364\text{molC}}{0.0104} = 3.5 \times 2 = 7\text{C}$$

$$0.0312\text{gH}\left(\frac{1\text{mol}}{1\text{g}}\right) = 0.0312\text{molH} \quad \frac{0.0312\text{molH}}{0.0104} = 3 \times 2 = 6\text{H}$$

Thus $\text{C}_7\text{H}_6\text{O}_2$

$$0.167\text{gO}\left(\frac{1\text{mol}}{16\text{g}}\right) = 0.0104\text{molO} \quad \frac{0.0104\text{molO}}{0.0104} = 1 \times 2 = 2\text{Oxy}$$

3. The combustion analysis of 19.8mg of an organic acid produced 39.6 mg of carbon dioxide and 16.2 mg of water. The molar mass is ~88 g/mole. Determine the molecular formula.

$$16.2\text{mgH}_2\text{O}\left(\frac{2\text{g}}{18\text{g}}\right) = 1.8\text{mgH} \quad 39.6\text{mgCO}_2\left(\frac{12\text{g}}{44\text{g}}\right) = 10.8\text{mgC} \quad 19.8\text{mgTotal} - 10.8\text{mgC} - 1.8\text{mgH} = 7.2\text{mgO}$$

$$10.8\text{mgC}\left(\frac{1\text{mmol}}{12\text{mg}}\right) = 0.90\text{mmolC} \quad \frac{0.90\text{mmolC}}{0.45} = 2\text{C}$$

$$1.8\text{mgH}\left(\frac{1\text{mmol}}{1\text{mg}}\right) = 1.8\text{mmolH} \quad \frac{1.8\text{mmolH}}{0.45} = 4\text{H}$$

Thus $\text{C}_2\text{H}_4\text{O}$

$$7.2\text{mgO}\left(\frac{1\text{mmol}}{16\text{mg}}\right) = 0.45\text{mmolO} \quad \frac{0.45\text{mmolO}}{0.45} = 1\text{Oxy}$$

The molar mass of the empirical formula is $\text{C}_2\text{H}_4\text{O} = 44 \frac{\text{g}}{\text{mol}} \quad \frac{88\text{g}}{44\text{mol}} = 2$ thus $\text{C}_4\text{H}_8\text{O}_2$

4. First calculate the mass of hydrogen and carbon. $19.96\text{mgH}_2\text{O}\left(\frac{2\text{g}}{18\text{g}}\right) = 2.218\text{mgH}$ $78.99\text{mgCO}_2\left(\frac{12\text{g}}{44\text{g}}\right) = 21.54\text{mgC}$

Then determine the mass of nitrogen $0.0462 \times 32\text{mg} = 1.478\text{mgN}$

Use the mass of C, H, and N to determine if there is any "missing" mass, which would be oxygen

$$32.00\text{mgTotal} - 21.54\text{mgC} - 2.218\text{mgH} - 1.478\text{mgN} = 6.764\text{mgO}$$

$$21.54\text{mgC}\left(\frac{1\text{mol}}{12\text{g}}\right) = 2.22\text{mmolC} \quad \frac{2.22\text{mmolC}}{0.106} = 16.9\text{C} \sim 17$$

$$2.218\text{mgH}\left(\frac{1\text{mol}}{1\text{g}}\right) = 2.218\text{mmolH} \quad \frac{2.218\text{mmolH}}{0.1057} = 20.9\text{H} \sim 21$$

$$1.48\text{mgN}\left(\frac{1\text{mol}}{14\text{g}}\right) = 0.106\text{mmolN} \quad \frac{0.106\text{mmolN}}{0.106} = 1\text{N}$$

Thus $\text{C}_{17}\text{H}_{21}\text{NO}_4$ which is indeed the chemical formula of cocaine.

$$6.764\text{mgO}\left(\frac{1\text{mol}}{16\text{g}}\right) = 0.423\text{mmolO} \quad \frac{0.423\text{mmolO}}{0.106} = 4\text{Oxy}$$