Percentage Composition and the Empirical Formula

Ibuprofen is a carbon-hydrogen-oxygen compound used in painkillers. When a 2.174-g sample is burned completely, it yields 6.029 g CO_2 and 1.709 g H_2O.

(**a**) What is the percent composition, by mass, of ibuprofen?
(**b**) What is the empirical formula of ibuprofen?

Solution:

Start by writing a model chemical equation:

$$C_xH_yO_z + O_2 \rightarrow x\,CO_2 + \frac{y}{2}H_2O$$

Realizing that the total amount, in moles, of carbon in the CO_2 formed comes from the ibuprofen as does the H in H_2O, it is possible to calculate quantities, in moles and grams, of both C and H:

$$n_\mathrm{C} = 6.029\text{ g CO}_2 \times \frac{1\text{ mol}}{44.01\text{ g}} \times \frac{1\text{ mol C}}{1\text{ mol CO}_2} = 0.13699\text{ mol C}$$

$$m_\mathrm{C} = 0.13699\text{ mol C} \times 12.01\tfrac{\text{g}}{\text{mol}} = 1.6453\text{ g C}$$

$$n_\mathrm{H} = 1.709\text{ g H}_2\text{O} \times \frac{1\text{ mol}}{18.015\text{ g}} \times \frac{2\text{ mol H}}{1\text{ mol H}_2\text{O}} = 0.18973\text{ mol H}$$

$$m_\mathrm{H} = 0.18973\text{ mol H} \times 1.00794\tfrac{\text{g}}{\text{mol}} = 0.19124\text{ g H}$$

Now that the masses of C and H in the 2.174 g sample are known, it's a simple matter to calculate the percentage composition of those two elements:

$$\%\text{C} = \frac{1.6453\text{ g C}}{2.174\text{ g ibuprofen}} \times 100 = \boxed{75.68\%\text{C}}$$

$$\%\text{H} = \frac{0.19124\text{ g H}}{2.174\text{ g ibuprofen}} \times 100 = \boxed{8.797\%\text{H}}$$

The text of the problem said that ibuprofen contains C, H, and O so the percentage composition oxygen is simply the remaining percentage:

$$\%\text{O} = 100 - \left(75.68\%\text{C} + 8.797\%\text{H}\right) = \boxed{15.52\%\text{O}}$$

Finally, use the simple algorithm for determining the empirical formula from percentage composition:

$\%C = 75.68\%C$

$\%H = 8.797\%H$

$\%O = 15.52\%O$

Assume 100 g of ibuprofen and convert the masses into molar quantities:

$$n_C = 75.68 \text{ g C} \Big/ 12.011 \tfrac{\text{g}}{\text{mol}} = 6.301 \text{ mol C}$$

$$n_H = 8.797 \text{ g H} \Big/ 1.0079 \tfrac{\text{g}}{\text{mol}} = 8.727 \text{ mol H}$$

$$n_C = 15.52 \text{ g O} \Big/ 16.00 \tfrac{\text{g}}{\text{mol}} = 0.970 \text{ mol O}$$

Normalize to 1 mol O by dividing each by 0.970 mol:

$n_C = 6.496 \text{ C}$

$n_H = 8.997 \text{ H}$

$n_C = 1.00 \text{ O}$

Normalize again to increase the fraction ~6.5 C by multiplying by 2:

$n_C = 13 \text{ C}$

$n_H = 18 \text{ H}$

$n_C = 2 \text{ O}$

$$\boxed{\text{Empirical formula} = C_{13}H_{18}O_2}$$