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$_2$O.

(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:

$$\text{C}_x\text{H}_y\text{O}_z + \text{O}_2 \rightarrow x \text{CO}_2 + \frac{y}{2} \text{H}_2\text{O}$$

Realizing that the total amount, in moles, of carbon in the CO$_2$ formed comes from the ibuprofen as does the H in H$_2$O, it is possible to calculate quantities, in moles and grams, of both C and H:

\[
\begin{align*}
n_C &= 6.029 \text{ g CO}_2 \times \frac{1 \text{ mol}}{44.01 \text{ g}} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} = 0.13699 \text{ mol C} \\
m_C &= 0.13699 \text{ mol C} \times 12.01 \text{ g/mol} = 1.6453 \text{ g C}
\end{align*}
\]

\[
\begin{align*}
n_H &= 1.709 \text{ g H}_2\text{O} \times \frac{1 \text{ mol}}{18.015 \text{ g}} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} = 0.18973 \text{ mol H} \\
m_H &= 0.18973 \text{ mol H} \times 1.00794 \text{ g/mol} = 0.19124 \text{ g H}
\end{align*}
\]

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:

\[
\begin{align*}
\%C &= \frac{1.6453 \text{ g C}}{2.174 \text{ g ibuprofen}} \times 100 = 75.68\% \text{C} \\
\%H &= \frac{0.19124 \text{ g H}}{2.174 \text{ g ibuprofen}} \times 100 = 8.797\% \text{H}
\end{align*}
\]

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

\[
\%O = 100 - (75.68\% \text{C} + 8.797\% \text{H}) = 15.52\% \text{O}
\]

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:

\[ n_C = \frac{75.68 \text{ g C}}{12.011 \frac{\text{g}}{\text{mol}}} = 6.301 \text{ mol C} \]
\[ n_H = \frac{8.797 \text{ g H}}{1.0079 \frac{\text{g}}{\text{mol}}} = 8.727 \text{ mol H} \]
\[ n_O = \frac{15.52 \text{ g O}}{16.00 \frac{\text{g}}{\text{mol}}} = 0.970 \text{ mol O} \]

Normalize to 1 mol O by dividing each by 0.970 mol:
\[ n_C = 6.496 \text{ C} \]
\[ n_H = 8.997 \text{ H} \]
\[ n_O = 1.00 \text{ O} \]

Normalize again to increase the fraction ~6.5 C by multiplying by 2:
\[ n_C = 13 \text{ C} \]
\[ n_H = 18 \text{ H} \]
\[ n_O = 2 \text{ O} \]

**Empirical formula = C_{13}H_{18}O_2**