Empirical and Molecular Formulas

**Empirical Formula:** The lowest whole number ratio between the elements in a compound (not necessarily the actual formula of the compound).

**Molecular Formula:** The actual formula of a molecular compound (the fixed ratio between the elements in the molecule).

Example: glucose

<table>
<thead>
<tr>
<th>molecular formula</th>
<th>empirical formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₆H₁₂O₆</td>
<td>CH₂O</td>
</tr>
</tbody>
</table>

- The empirical formula is useful because it can be determined experimentally from the percent composition by mass or from the combustion products (see following pages).
- The molecular formula can be found from the empirical formula using the scaling factor if the molar mass of the compound is known (the molar mass can also be determined experimentally).

Scaling Factor = \( \frac{\text{molar mass of compound}}{\text{molar mass of empirical formula}} \)

Example: The molar mass of a compound with the empirical formula CH₂O is 180.156 g/mol. What is the molecular formula of the compound?

Scaling Factor = \( \frac{\text{mass compound}}{\text{mass CH}_2\text{O}} \) = \( \frac{180.156 \text{ g/mol}}{30.026 \text{ g/mol}} \) = 6

CH₂O = 1(12.01 g/mol) + 2(1.008 g/mol) + 1(16.00 g/mol)

\[ \begin{align*}
\text{CH}_2\text{O} & \quad \text{\( \leftarrow \) empirical formula} \\
\times 6 & \quad \text{\( \leftarrow \) multiply subscripts by scaling factor} \\
\text{C}_6\text{H}_{12}\text{O}_6 & \quad \text{\( \leftarrow \) molecular formula}
\end{align*} \]

Molecular formula = C₆H₁₂O₆
Calculating the empirical and molecular formulas from the percent composition by mass and the molar mass of the compound:

Steps:
- Assume that you have a 100.0 gram sample of the compound. The percent by mass would then be the mass (in grams) you have of each element.
- Convert grams of each element to moles using the molar mass.
- Divide all moles by the least number of moles.
- If any resulting number is not a whole number, multiply through by the smallest number that would make the fractions whole numbers.
- These whole numbers are the subscripts in the empirical formula.
- Use the molar mass of the compound to determine the scaling factor, and scale the empirical formula up to the molecular formula.

Example: A compound is 43.7% P, and 56.3% O by mass, and has a molar mass of 283.88 g/mol. What are the empirical and molecular formulas?

Assume a 100.0 g sample of the compound:

\[
\begin{align*}
\text{P} & \quad 43.7 \text{ g P} \quad \left( \frac{1 \text{ mol P}}{30.97 \text{ g P}} \right) = 1.41 \text{ mol P} \\
\text{O} & \quad 56.3 \text{ g O} \quad \left( \frac{1 \text{ mol O}}{16.00 \text{ g O}} \right) = 3.52 \text{ mol O}
\end{align*}
\]

\[
\begin{align*}
\text{Divide all moles by the least number of moles:} \\
\quad \text{P:} \quad \frac{1.41 \text{ mol}}{1.41 \text{ mol}} = 1.00 \\
\quad \text{O:} \quad \frac{3.52 \text{ mol}}{1.41 \text{ mol}} = 2.50
\end{align*}
\]

\[
\begin{align*}
\text{Multiply subscripts by scaling factor:} \\
\quad \text{P:} \quad 1.00 \times 2 = 2 \\
\quad \text{O:} \quad 2.50 \times 2 = 5
\end{align*}
\]

\[
\text{Empirical formula = P}_2\text{O}_5
\]

Scaling Factor = \( \frac{\text{mass compound}}{\text{mass P}_2\text{O}_5} \) = \( \frac{283.88 \text{ g/mol}}{141.94 \text{ g/mol}} \) = 2

\[
\text{P}_2\text{O}_5 = 2(30.97 \text{ g/mol}) + 5(16.00 \text{ g/mol})
\]

\[
\text{P}_2\text{O}_5 \quad \leftarrow \text{empirical formula} \\
\times 2 \quad \leftarrow \text{multiply subscripts by scaling factor} \\
\text{P}_4\text{O}_{10} \quad \leftarrow \text{molecular formula}
\]

\[
\text{Molecular formula = P}_4\text{O}_{10} \quad \text{(tetraphosphorus decoxide)}
\]
Determining the empirical & molecular formulas from combustion products and the molar mass of the compound:

- All the Carbon is converted to CO$_2$
- All the Hydrogen is converted to H$_2$O
- If there is a third element present it is the balance of the mass
- Combustion Problem Flow Chart:

\[
\text{g CO}_2 \quad \rightarrow \quad \text{mol CO}_2 \quad \rightarrow \quad \text{mol C} \quad \rightarrow \quad \text{g C} \\
\text{g H}_2\text{O} \quad \rightarrow \quad \text{mol H}_2\text{O} \quad \rightarrow \quad \text{mol H} \quad \rightarrow \quad \text{g H} \\
\text{g O} \quad \rightarrow \quad \text{mol O} \quad \rightarrow \quad \text{need for emp. formula} \quad \rightarrow \quad \text{subtract from mass of compound to get g O}
\]

Example: A sample contains only C, H, & O. Combustion of 10.68 mg of sample yields 16.01 mg CO$_2$ and 4.37 mg H$_2$O. The molar mass of the compound is 176.1 g/mol. What are the empirical and molecular formulas?

\[
\begin{align*}
\text{g CO}_2 \quad \rightarrow \quad \text{mol CO}_2 \quad \rightarrow \quad \text{mol C} \quad \rightarrow \quad \text{g C} \\
16.01 \text{ mg CO}_2 \quad \left( \frac{1 \text{ mmol CO}_2}{44.01 \text{ mg CO}_2} \right) \quad \left( \frac{1 \text{ mmol C}}{1 \text{ mmol CO}_2} \right) = 0.36378 \text{ mmol C} \\
16.01 \text{ mg CO}_2 \quad \left( \frac{12.01 \text{ mg C}}{1 \text{ mmol C}} \right) = 4.369 \text{ mg C}
\end{align*}
\]

\[
\begin{align*}
\text{g H}_2\text{O} \quad \rightarrow \quad \text{mol H}_2\text{O} \quad \rightarrow \quad \text{mol H} \quad \rightarrow \quad \text{g H} \\
4.37 \text{ mg H}_2\text{O} \quad \left( \frac{1 \text{ mmol H}_2\text{O}}{18.016 \text{ mg H}_2\text{O}} \right) \quad \left( \frac{2 \text{ mmol H}}{1 \text{ mmol H}_2\text{O}} \right) = 0.48512 \text{ mmol H} \\
4.37 \text{ mg H}_2\text{O} \quad \left( \frac{1.008 \text{ mg H}}{1 \text{ mmol H}} \right) = 0.489 \text{ mg H}
\end{align*}
\]

\[
\begin{align*}
\text{10.68 mg total} \\
- 4.369 \text{ mg C} \\
- 0.489 \text{ mg H} \\
= 5.822 \text{ mg O}
\end{align*}
\]
From previous steps:

\[
\begin{align*}
0.36378 \text{ mmol C} & \quad = 1.000 \quad = 3 \\
0.48512 \text{ mmol H} & \div 0.36378 \text{ mmol} \quad = 1.33 \quad \times 3 \quad = 4 \\
5.822 \text{ mg O} \left( \frac{1 \text{ mmol O}}{16.00 \text{ mg O}} \right) & = 0.36387 \text{ mmol O} \quad = 1.00 \quad = 3 \\
\end{align*}
\]

**Empirical formula** = \( \text{C}_3\text{H}_4\text{O}_3 \)

Scaling Factor = \( \frac{\text{mass compound}}{\text{mass } \text{C}_3\text{H}_4\text{O}_3} \) = \( \frac{176.1 \text{ g/mol}}{88.062 \text{ g/mol}} \) = 2

\( \text{C}_3\text{H}_4\text{O}_3 = 3(12.01 \text{ g/mol}) + 4(1.008 \text{ g/mol}) + 3(16.00 \text{ g/mol}) = 88.062 \text{ g/mol} \)

\( \begin{align*}
\text{C}_3\text{H}_4\text{O}_3 \quad & \leftarrow \text{empirical formula} \\
\times 2 \quad & \leftarrow \text{multiply subscripts by scaling factor} \\
\text{C}_6\text{H}_8\text{O}_6 \quad & \leftarrow \text{molecular formula}
\end{align*} \)

**Molecular formula** = \( \text{C}_6\text{H}_8\text{O}_6 \)