**Percent Composition**

- Percent composition is the expression of relative amounts of elements present in a sample, given as percentages.

- Determination of percent composition can be done from two starting points:
  1. from a given formula
  2. from mass data given in the problem (if formula is not known)

- It’s important to remember:

\[
\% = \frac{\text{part}}{\text{whole}} \times 100
\]

**Steps for Determining Percent Composition:**

1. If necessary) Calculate the molar mass of the compound.
   
   This is done if you are given a formula to start with.

2. For each component you wish to analyze, do the following:

   \[
   \text{Calculate percent by dividing} \frac{\text{element mass}}{\text{total mass}} \times 100
   \]

3. Check your work by ensuring percentages of all elements total 100%.
% Composition of Aspirin

A 500.00 mg tablet of aspirin contains 300.0 mg of carbon, and 22.5 mg of hydrogen. The rest is oxygen. What is the percent composition of aspirin?

C: \( \frac{300.0 \text{ mg}}{500.00 \text{ mg}} \times 100 = 60\% \) C

H: \( \frac{22.5 \text{ mg}}{500.00 \text{ mg}} \times 100 = 4.5\% \) H

O: \( 500 - (300.0 + 22.5) = \frac{177.5 \text{ mg}}{500.00 \text{ mg}} \times 100 = 35.5\% \) O

Aspirin is often taken with a sip of water. What is the percent composition of water?

\[
\text{water} = H_2O \quad \text{molar mass} = 2(1.008) + 15.99 = 18.006 \text{ g/mol}
\]

H: \( 2 \times 1.008 = \frac{2.016}{18.006} \times 100 = 11.2\% \)

O: \( 1 \times 15.99 = \frac{15.99}{18.006} \times 100 = 88.97\% \)

Empirical formula of Aspirin

Based on the percent composition values determined on the previous page, calculate the empirical formula of aspirin.

C: \( 60\% \rightarrow \frac{6.0 \text{ g}}{12.01 \text{ g/mol}} = \frac{1 \text{ mol}}{12.01 \text{ g}} = 4.996 \text{ mol} \rightarrow \frac{4.996 \text{ mol}}{2.21} = 2.25 \rightarrow 2.25 \times 4 = 9 \)

H: \( 4.5\% \rightarrow \frac{4.5 \text{ g}}{1.008 \text{ g/mol}} = \frac{1 \text{ mol}}{1.008 \text{ g/mol}} = 4.46 \text{ mol} \rightarrow \frac{4.46 \text{ mol}}{2.21} = 2 \rightarrow 2 \times 4 = 8 \)

O: \( 33.5\% \rightarrow \frac{33.5 \text{ g}}{16.00 \text{ g/mol}} = \frac{1 \text{ mol}}{16.00 \text{ g/mol}} = 2.21 \text{ mol} \rightarrow \frac{2.21 \text{ mol}}{2.21} = 1 \rightarrow 1 \times 4 = 4 \)

ans: \( C_9H_8O_4 \)

Based on the mass values of the components of aspirin given on the previous page, calculate the empirical formula of aspirin.

C: \( \frac{300 \text{ mg}}{12.01 \text{ g/mol}} = 24.98 \text{ mol} \rightarrow \frac{24.98}{11.09} = 2.25 \times 4 = 9 \)

H: \( \frac{22.5 \text{ mg}}{1.008 \text{ g/mol}} = 22.32 \text{ mol} \rightarrow \frac{22.32}{11.09} = 2 \times 4 = 8 \)

O: \( \frac{17.25 \text{ mg}}{16.00 \text{ g/mol}} = 11.09 \text{ mol} \rightarrow \frac{11.09}{11.09} = 1 \times 4 = 4 \)
**Empirical Formulas**

- An empirical formula is the expression of the formula of a compound as the smallest whole-number ratio of atoms.

  Example: The empirical formula of H$_2$O$_2$ is HO

- Determination of empirical formulas from data can be done from two starting points:
  1. masses of component elements
  2. percent of component elements

**REMEMBER** that subscripts are just ratios.

**Steps for Determining Empirical Formulas:** (Rhyme style)

1. **Percent to mass**
   If necessary, convert % to mass by: assuming 100 g and changing percent to g

2. **Mass to moles**
   Convert mass to moles by: dividing by molar mass

3. **Divide by small**
   Divide all moles by the smallest to establish ratios

4. **Multiply 'til whole**
   **Only do this if you have decimals - otherwise stop at step 3!!**
   Multiply all ratios by some whole number to get whole numbers

**Molecular Formulas**

- A molecular formula is the expression of the formula of a compound as it is actually found in nature.

  Circle the molecular formulas: H$_2$O, CH, C$_6$H$_{12}$O$_6$, OH

- Determination of molecular formulas often happen in conjunction with the determination of empirical formulas (which is why the steps below start at step 5).

  * sometimes the molecular and empirical formulas are the same!!!!

**IMPORTANT NOTE:** A molecular mass must be given for the unknown compound.

**Steps for Determining Molecular Formulas:**

5. **Determine the molar mass of the empirical formula first.**

6. **Divide the molecular mass by the empirical mass to get a ratio** (should always get a whole #)

7. **Multiply** the subscripts of the empirical formula by this ratio
MOLECULAR FORMULA OF CAFFEINE

Some aspirin tablets (such as Anacin) also contain caffeine, as this helps many people get rid of a headache faster and more effectively. Caffeine has the following percent composition: carbon 49.48%, hydrogen 5.19%, oxygen 16.48% and nitrogen 28.85%. Its molecular weight is 194.19 g/mol. What is its molecular formula? What is the empirical formula?

\[
\begin{align*}
\text{C: } 49.48\% & \rightarrow \frac{49.48 \text{ g}}{12.01 \text{ g/mol}} \times \frac{1 \text{ mol}}{1 \text{ mol}} = 4.12 \text{ mol} \rightarrow \frac{4.12 \text{ mol}}{1.03} = 4 \\
\text{H: } 5.19\% & \rightarrow \frac{5.19 \text{ g}}{1.008 \text{ g/mol}} \times \frac{1 \text{ mol}}{1 \text{ mol}} = 5.15 \text{ mol} \rightarrow \frac{5.15 \text{ mol}}{1.03} = 5 \\
\text{O: } 16.48\% & \rightarrow \frac{16.48 \text{ g}}{16 \text{ g/mol}} \times \frac{1 \text{ mol}}{1 \text{ mol}} = 1.03 \text{ mol} \rightarrow \frac{1.03 \text{ mol}}{1.03} = 1 \\
\text{N: } 28.5\% & \rightarrow \frac{28.5 \text{ g}}{14.01 \text{ g/mol}} \times \frac{1 \text{ mol}}{1 \text{ mol}} = 2.06 \text{ mol} \rightarrow \frac{2.06 \text{ mol}}{1.03} = 2
\end{align*}
\]

\[
(4 \times 12.01) + (5 \times 1.008) + (1 \times 16.01) + (2 \times 14.01) = 97.12
\]

\[
\text{molecular} = \frac{194.19}{97.12} = 2 \\
\text{empirical} = \frac{194.19}{194.19} = 1
\]

\[
\begin{align*}
\text{molecular} & = \frac{194.19}{97.12} = 2 \\
\text{empirical} & = \frac{194.19}{194.19} = 1
\end{align*}
\]

C_{4}H_{10}O_{2}N_{4}