Chapter 3: Stoichiometry

Key Skills:
- Balance chemical equations
- Predict the products of simple combination, decomposition, and combustion reactions.
- Calculate formula weights
- Convert grams to moles and moles to grams using molar masses.
- Convert number of molecules to moles and moles to number of molecules using Avogadro's number
- Calculate the empirical and molecular formulas of a compound from percentage composition and molecular weight.
- Identify limiting reactants and calculate amounts, in grams or moles, or reactants consumed and products formed for a reaction.
- Calculate the percent yield of a reaction.

Stoichiometry is the study of the quantitative relationships in substances and their reactions
- Chemical equations
- The mole and molar mass
- Chemical formulas
- Mass relationships in equations
- Limiting reactant
Definitions

- **Reactants** are the substances consumed
- **Products** are the substances formed
- **Coefficients** are numbers before the formula of a substance in an equation
- A **balanced** equation has the same number of atoms of each element on both sides of the equation

Chemical Equations

- A chemical equation is a shorthand notation to describe a chemical reaction
  - Just like a chemical formula, a chemical equation expresses quantitative relations
- Subscripts tell the number of atoms of each element in a molecule
- Coefficients tell the number of molecules

\[ \text{Reactants} \quad 2\text{H}_2 + \text{O}_2 \quad \rightarrow \quad \text{Products} \quad 2\text{H}_2\text{O} \]
Hydrogen and oxygen can make water or hydrogen peroxide

\[ 2 \text{H}_2(g) + \text{O}_2(g) \rightarrow 2 \text{H}_2\text{O}(l) \]
\[ \text{H}_2(g) + \text{O}_2(g) \rightarrow \text{H}_2\text{O}_2(l) \]
Anatomy of a Chemical Equation

Reactants appear on the left side of the equation. Products appear on the right side of the equation.

The states of the reactants and products are written in parentheses to the right of each element symbol or formula.

Writing Balanced Equations

- Write the correct formula for each substance
  \[ \text{H}_2 + \text{Cl}_2 \rightarrow \text{HCl} \]
- Add coefficients so the number of atoms of each element are the same on both sides of the equation
  \[ \text{H}_2 + \text{Cl}_2 \rightarrow 2\text{HCl} \]
Balancing Chemical Equations

• Assume one molecule of the most complicated substance
  \[ \text{C}_5\text{H}_{12} + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]

• Adjust the coefficient of \( \text{CO}_2 \) to balance C
  \[ \text{C}_5\text{H}_{12} + \text{O}_2 \rightarrow 5\text{CO}_2 + \text{H}_2\text{O} \]

• Adjust the coefficient of \( \text{H}_2\text{O} \) to balance H
  \[ \text{C}_5\text{H}_{12} + \text{O}_2 \rightarrow 5\text{CO}_2 + 6\text{H}_2\text{O} \]

• Adjust the coefficient of \( \text{O}_2 \) to balance O
  \[ \text{C}_5\text{H}_{12} + 8\text{O}_2 \rightarrow 5\text{CO}_2 + 6\text{H}_2\text{O} \]

• Check the balance by counting the number of atoms of each element.

Balancing Equations

• Sometimes fractional coefficients are obtained
  \[ \text{C}_5\text{H}_{10} + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]

  \[ \text{C}_5\text{H}_{10} + \text{O}_2 \rightarrow 5\text{CO}_2 + \text{H}_2\text{O} \]

  \[ \text{C}_5\text{H}_{10} + \text{O}_2 \rightarrow 5\text{CO}_2 + 5\text{H}_2\text{O} \]

  \[ \text{C}_5\text{H}_{10} + \left( \frac{15}{2} \right) \text{O}_2 \rightarrow 5\text{CO}_2 + 5\text{H}_2\text{O} \]

• Multiply all coefficients by the denominator
  \[ 2 \text{C}_5\text{H}_{10} + 15 \text{O}_2 \rightarrow 10\text{CO}_2 + 10\text{H}_2\text{O} \]
Combination

Two or more reactants combine to form a single product. Many elements react with one another in this fashion to form compounds.

Combination Reactions

<table>
<thead>
<tr>
<th>A + B → C</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(s) + O₂(g) → CO₂(g)</td>
</tr>
<tr>
<td>N₂(g) + 3H₂(g) → 2NH₃(g)</td>
</tr>
<tr>
<td>CaO(s) + H₂O(l) → Ca(OH)₂(aq)</td>
</tr>
</tbody>
</table>

Decomposition

One substance breaks down into two or more substances

| 2 NaN₃(s) → 2 Na(s) + 3 N₂(g) |
| CaCO₃(s) → CaO(s) + CO₂(g) |
| 2 KClO₃(s) → 2 KCl(s) + O₂(g) |

Decomposition Reactions

<table>
<thead>
<tr>
<th>C → A + B</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 KClO₃(s) → 2 KCl(s) + 3 O₂(g)</td>
</tr>
<tr>
<td>PbCO₃(s) → PbO(s) + CO₂(g)</td>
</tr>
<tr>
<td>Cu(OH)₂(s) → CuO(s) + H₂O(g)</td>
</tr>
</tbody>
</table>

A single reactant breaks apart to form two or more substances. Many compounds react this way when heated.
Combustion

Is the process of burning, the combination of an organic substance with oxygen to produce a flame.

- When an organic compound burns in oxygen, the carbon reacts with oxygen to form $\text{CO}_2$, and the hydrogen forms water, $\text{H}_2\text{O}$.

Balance the following combustion reactions:

$$\text{C}_3\text{H}_8 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$$

$$\text{(C}_2\text{H}_5)_2\text{O} + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$$

Formula Weight (FW)

- Sum of the atomic weights for the atoms in a chemical formula
- The formula weight of calcium chloride, $\text{CaCl}_2$, would be
  $\text{Ca: } 1(40.08 \text{ amu})$
  $+ \text{Cl: } 2(35.45 \text{ amu})$
  $110.98 \text{ amu}$
- Formula weights are generally reported for ionic compounds
Molecular Weight (MW)

- Sum of the atomic weights of the atoms in a molecule
- For the molecule ethane, $\text{C}_2\text{H}_6$, the molecular weight would be

\[
\text{C: } 2(12.01 \text{ amu}) \\
+ \text{H: } 6(1.008 \text{ amu}) \\
\text{30.07 amu}
\]

Percent Composition

One can find the percentage of the mass of a compound that comes from each of the elements in the compound by using this equation:

\[
\% \text{ element} = \frac{\text{(number of atoms)(atomic weight)}}{\text{(FW of the compound)}} \times 100\%
\]
Percent Composition

So the percentage by mass of carbon in ethane ($C_2H_6$) is...

$$\%C = \frac{(2)(12.01 \text{ amu})}{(30.068 \text{ amu})} \times 100$$

$$= \frac{24.02 \text{ amu}}{30.068 \text{ amu}} \times 100$$

$$= 79.89\%$$

The Mole

- One **mole** is the amount of substance that contains as many entities as the number of atoms in exactly 12 grams of the $^{12}\text{C}$ isotope of carbon.
- **Avogadro’s number** is the experimentally determined number of atoms in 12 g of isotopically pure $^{12}\text{C}$, and is equal to $6.022 \times 10^{23}$
- One mole of anything contains $6.022 \times 10^{23}$ entities

- 1 mol H = $6.022 \times 10^{23}$ atoms of H
- 1 mol $H_2$ = $6.022 \times 10^{23}$ molecules of $H_2$
- 1 mol CH$_4$ = $6.022 \times 10^{23}$ molecules of CH$_4$
- 1 mol CaCl$_2$ = $6.022 \times 10^{23}$ formula units of CaCl$_2$
Moles to Number of Entities

<table>
<thead>
<tr>
<th>Moles of substance</th>
<th>Avogadro's number</th>
<th>Number of atoms or molecules</th>
</tr>
</thead>
</table>

**Example Calculations**

- How many Na atoms are present in 0.35 mol of Na?
- How many moles of C₂H₆ are present in 3.00 \times 10^{21} molecules of C₂H₆?

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**TABLE 3.2 Mole Relationships**

<table>
<thead>
<tr>
<th>Name of Substance</th>
<th>Formula</th>
<th>Formula Weight (amu)</th>
<th>Molar Mass (g/mol)</th>
<th>Number and Kind of Particles in One Mole</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic nitrogen</td>
<td>N</td>
<td>14.0</td>
<td>14.0</td>
<td>6.02 \times 10^{23} N atoms</td>
</tr>
<tr>
<td>Molecular nitrogen or “dinitrogen”</td>
<td>N₂</td>
<td>28.0</td>
<td>28.0</td>
<td>{ 6.02 \times 10^{23} N₂ molecules, 2(6.02 \times 10^{23}) N atoms }</td>
</tr>
<tr>
<td>Silver</td>
<td>Ag</td>
<td>107.9</td>
<td>107.9</td>
<td>6.02 \times 10^{23} Ag atoms</td>
</tr>
<tr>
<td>Silver ions</td>
<td>Ag⁺</td>
<td>107.9¹</td>
<td>107.9</td>
<td>6.02 \times 10^{23} Ag⁺ ions</td>
</tr>
<tr>
<td>Barium chloride</td>
<td>BaCl₂</td>
<td>208.2</td>
<td>208.2</td>
<td>{ 6.02 \times 10^{23} BaCl₂ formula units, 6.02 \times 10^{23} Ba^{2+} ions, 2(6.02 \times 10^{23}) Cl⁻ ions }</td>
</tr>
</tbody>
</table>

¹Recall that the mass of an electron is more than 1800 times smaller than the masses of the proton and the neutron; thus, ions and atoms have essentially the same mass.
# Molar Mass

The **molar mass** \( (M) \) of any atom, molecule or compound is the mass (in grams) of one mole of that substance.

The molar mass in grams is numerically equal to the atomic mass or molecular mass expressed in u (or amu).

<table>
<thead>
<tr>
<th>Substance</th>
<th>Name</th>
<th>Mass</th>
<th>Molar Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>atomic mass</td>
<td>39.95 u</td>
<td>39.95 g/mol</td>
</tr>
<tr>
<td>C(_2)H(_6)</td>
<td>molecular mass</td>
<td>30.07 u</td>
<td>30.07 g/mol</td>
</tr>
<tr>
<td>NaF</td>
<td>formula mass</td>
<td>41.99 u</td>
<td>41.99 g/mol</td>
</tr>
</tbody>
</table>

What mass of compound must be weighed out, to have a 0.0223 mol sample of H\(_2\)C\(_2\)O\(_4\) \((M = 90.04 \text{ g/mol})\)?
Interconverting masses and number of formula units

Example Calculation

What is the mass of 0.25 moles of CH$_4$?

$$0.25 \text{ mol} \cdot \text{CH}_4 \left( \frac{16.0 \text{ g CH}_4}{1 \text{ mol CH}_4} \right) = 4.0 \text{ g CH}_4$$

Empirical formula

Example 1: What is the empirical formula of a compound that contains 0.799 g C and 0.201 g H in a 1.000 g sample?

Example 2: What is the empirical formula of a chromium oxide that is 68.4% Cr by mass?
Combustion Analysis

Compounds containing C, H and O are routinely analyzed through combustion in a chamber like this:
- C is determined from the mass of CO₂ produced
- H is determined from the mass of H₂O produced
- O is determined by difference after the C and H have been determined

Finding C and H content

A weighed sample of compound is burned, and the masses of H₂O and CO₂ formed is measured.
Calculating Empirical Formulas

Example: The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

Assuming 100.00 g of *para*-aminobenzoic acid,

\[
\begin{align*}
\text{C:} & \quad 61.31 \text{ g} \times \frac{1 \text{ mol}}{12.01 \text{ g}} = 5.105 \text{ mol C} \\
\text{H:} & \quad 5.14 \text{ g} \times \frac{1 \text{ mol}}{1.01 \text{ g}} = 5.09 \text{ mol H} \\
\text{N:} & \quad 10.21 \text{ g} \times \frac{1 \text{ mol}}{14.01 \text{ g}} = 0.7288 \text{ mol N} \\
\text{O:} & \quad 23.33 \text{ g} \times \frac{1 \text{ mol}}{16.00 \text{ g}} = 1.456 \text{ mol O}
\end{align*}
\]

Calculate the mole ratio by dividing by the smallest number of moles:

\[
\begin{align*}
\text{C:} & \quad \frac{5.105 \text{ mol}}{0.7288 \text{ mol}} = 7.005 \approx 7 \\
\text{H:} & \quad \frac{5.09 \text{ mol}}{0.7288 \text{ mol}} = 6.984 \approx 7 \\
\text{N:} & \quad \frac{0.7288 \text{ mol}}{0.7288 \text{ mol}} = 1.000 \\
\text{O:} & \quad \frac{1.458 \text{ mol}}{0.7288 \text{ mol}} = 2.001 \approx 2
\end{align*}
\]

The empirical formula of PABA is \(\text{C}_7\text{H}_7\text{NO}_2\).
**Example Calculation**

A compound contains only C, H, and O. A 0.1000 g sample burns completely in oxygen to form 0.0930 g water and 0.2271 g CO₂. Calculate the mass of each element in this sample. What is the empirical formula of the compound?
Mole Relationships in Equations

Guidelines for Reaction Stoichiometry

- Write the balanced equation.
- Calculate the number of moles of the species for which the mass is given.
- Use the coefficients in the equation to convert the moles of the given substance into moles of the substance desired.
- Calculate the mass of the desired species.
Given the reaction

$$4\text{FeS}_2 + 11 \text{O}_2 \rightarrow 2\text{Fe}_2\text{O}_3 + 8\text{SO}_2$$

What mass of SO$_2$ is produced from reaction of 3.8 g of FeS$_2$ and excess O$_2$?

**Example Calculation**

What mass of SO$_3$ forms from the reaction of 4.1 g of SO$_2$ with an excess of O$_2$?
Reaction Yields

**Actual yield** is found by measuring the quantity of product formed in the experiment.

**Theoretical yield** is calculated from reaction stoichiometry.

\[
\% \text{ yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%
\]

**Example: Calculating Percent Yield**

A 10.0 g-sample of potassium bromide is treated with perchloric acid solution. The reaction mixture is cooled and solid KClO\(_4\) is removed by filtering, then it is dried and weighed.

\[\text{KBr (aq)} + \text{HClO}_4 \text{(aq)} \rightarrow \text{KClO}_4 \text{(s)} + \text{HBr (aq)}\]

The product weighed 8.8 g. What was the percent yield?
Limiting Reactant

*Limiting reactant*: the reactant that is completely consumed in a reaction. When it is used up, the reaction stops, thus limiting the quantities of products formed.

*Excess reactant*: the other reactants present, not completely consumed.

\[2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g})\]
$2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g})$

Before reaction

After reaction

$5[2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g})]$

$10\text{H}_2(\text{g}) + 5\text{O}_2(\text{g}) \rightarrow 10\text{H}_2\text{O}(\text{g})$

$2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g})$

Before reaction

After reaction

$5[2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g})]$

$10\text{H}_2(\text{g}) + 5\text{O}_2(\text{g}) \rightarrow 10\text{H}_2\text{O}(\text{g})$
Strategy for Limiting Reactant

\[ 2 \text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2 \text{H}_2\text{O}(\text{g}) \]

<table>
<thead>
<tr>
<th></th>
<th>Before reaction:</th>
<th>Change (reaction):</th>
<th>After reaction:</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Moles of A} )</td>
<td>10 mol</td>
<td>−10 mol</td>
<td>0 mol</td>
</tr>
<tr>
<td>( \text{Moles of B} )</td>
<td>7 mol</td>
<td>−5 mol</td>
<td>2 mol</td>
</tr>
<tr>
<td>( \text{Molar mass of A} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \text{Molar mass of B} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \text{Molar mass of product} )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Example Calculation

Calculate the theoretical yield (g) when 7.0 g of N₂ reacts with 2.0 g of H₂, forming NH₃.

One reaction step in the conversion of ammonia to nitric acid involves converting NH₃ to NO by the following reaction:

\[ 4 \text{NH}_3(g) + 5 \text{O}_2(g) \rightarrow 4 \text{NO}(g) + 6 \text{H}_2\text{O}(g) \]

If 1.50 g of NH₃ reacts with 2.75 g O₂, then:

1. Which is the limiting reactant?
2. How many grams of NO and H₂O form?
3. How many grams of the excess reactant remain after the limiting reactant is completely consumed?
4. Is the law of conservation of mass obeyed?