Chapter 3
Chemical Reactions and Reaction Stoichiometry

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Formula Weight (FW)

• Sum of the atomic weights for the atoms in a chemical formula.
• Combines information from the chemical formula with atomic weights from the periodic table
• **Example:** The formula weight of calcium chloride, \( \text{CaCl}_2 \), is calculated as follows

\[
\begin{align*}
\text{Ca: } & \quad 1(40.08 \text{ amu}) = 40.08 \text{ amu Ca} \\
\text{Cl: } & \quad 2(35.45 \text{ amu}) = \frac{70.90 \text{ amu Cl}}{110.99 \text{ amu CaCl}_2}
\end{align*}
\]
Molecular Weight (MW)

- The formula weight of a molecular substance
- Equal the sum of the atomic weights of the atoms in a molecule; gives the total mass of one molecule of the substance

**Example:** The molecular weight of the molecule ethane, C₂H₆, would be calculated as follows:

\[
\begin{align*}
\text{C:} & \quad 2(12.01 \text{ amu}) = 24.02 \text{ amu C} \\
\text{H:} & \quad 6(1.01 \text{ amu}) = \frac{6.06 \text{ amu H}}{30.08 \text{ amu C}_2\text{H}_6}
\end{align*}
\]
Ionic Compounds and Formula Weights

- Ionic compounds exist with a three-dimensional crystal lattice of ions. So there is no simple group of atoms to call a molecule.

- Thus, ionic compounds are represented by empirical formulas and formula weights (not molecular weights).

- The formula weight of an ionic compound corresponds to the mass of one formula unit of that compound (or the combined mass of the smallest combination of cations and anions that is net neutral).

Click here to view a video tutorial that distinguishes between atomic weights, formula weights, and molecular weights.
Percent Composition (by Mass) of An Element in a Compound

% Mass Element = \frac{\text{(mass of element in sample of compound)}}{\text{(total mass of sample)}} \times 100

Click here to view a tutorial video on percent composition (by mass).
Determining Percent Composition Based on the Chemical Formula of a Compound

\[
\text{% Element} = \frac{\text{(number of atoms in formula)} \times \text{(atomic weight)}}{\text{(FW of the compound)}} \times 100
\]

**Example:** Determine the mass-percentage of carbon in ethane (\(\text{C}_2\text{H}_6\)). (Recall from slide 3 that \(\text{FW}_{\text{ethane}} = 30.08\ \text{amu}\))

\[
\%\text{C} = \frac{(2)(12.01\ \text{amu})}{(30.08\ \text{amu})} \times 100
\]

\[
= \frac{24.02\ \text{amu}}{30.08\ \text{amu}} \times 100
\]

\[
= 79.85\%
\]
Avogadro’s Number and the Mole:

A mole is Avogadro’s number of things.

- There are $6.022 \times 10^{23}$ atoms in 12.00 g of $^{12}$C. The former quantity is known as Avogadro’s number and is the basis for the SI unit of amount, the mole (mol):

  $$1 \text{ mole} = 6.022 \times 10^{23}$$

- Even a small sample of a substance contains an incredibly large number of atoms or molecules. So the mole is a convenient unit for expressing the amount of atoms or molecules in a typical chemical sample.

Click here to view an entertaining and educational animated video on the mole concept in chemistry.
**Molar Mass:** the mass of 1 mol of a substance (g/mol).

- **Note:** the molar mass of an atomic element (in g/mol) has the same numerical value as its atomic weight (in amu).

- **Note:** likewise, the molar mass of a molecule or ionic compound (in g/mol) has the same numerical value as its formula weight (in amu).

Click here to view a tutorial on calculating molar masses.
Mole Relationships

- One mole of atoms, ions, or molecules contains Avogadro’s number of those particles.
- Regarding the number of atoms of a given element in a substance: one mole of the substance contains Avogadro’s number times the number of atoms or ions of that element in the chemical formula for the substance.

### 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</td>
<td>N$_2$</td>
<td>28.0</td>
<td>28.0</td>
<td>{ $6.02 \times 10^{23}$ N$_2$ 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>107.9$^a$</td>
<td>107.9</td>
<td>$6.02 \times 10^{23}$ Ag$^+$ ions</td>
</tr>
<tr>
<td>Barium chloride</td>
<td>BaCl$_2$</td>
<td>208.2</td>
<td>208.2</td>
<td>{ $6.02 \times 10^{23}$ BaCl$_2$ formula units, 6.02 $\times 10^{23}$ Ba$^{2+}$ ions, 2(6.02 $\times 10^{23}$) Cl$^{-}$ ions }</td>
</tr>
</tbody>
</table>

$^a$Recall 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.
Mass-Moles-Number Calculations

- The mole unit provides a bridge between the molecular (submicroscopic) scale and the real-world (macroscopic) scale.
- Avogadro’s number allows us to convert between the number of moles (of atoms or molecules) and the number of individual particles.

Click here to view a tutorial on mass-mole conversion problems involving atoms. Also reviews the mole concept in chemistry.

Click here to view a tutorial on converting between the mass, the moles of atoms, and the number individual atoms in a sample of an element.
Click here to view a tutorial video on mass-mole-number of individual particle conversions for both atoms and molecules.
Determining Empirical Formulas from Percent-Mass Data

Outline of General strategy:

1. Given: Mass % elements
2. Assume 100-g sample
3. Grams of each element
4. Use molar mass
5. Moles of each element
6. Calculate mole ratio
7. Find: Empirical formula

Example: The compound \textit{para}-aminobenzoic acid (often listed as PABA on a 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.  \textit{(Note: all percentages are by mass.)}
Solution to Example Empirical Formula Problem

**Step 1:** Assuming 100.00 g of PABA, change each percent into grams, and convert grams to moles of each element:

C: $61.31 \text{ g} \times \frac{1 \text{ mol}}{12.01 \text{ g}} = 5.105 \text{ mol C}$

H: $5.14 \text{ g} \times \frac{1 \text{ mol}}{1.01 \text{ g}} = 5.09 \text{ mol H}$

N: $10.21 \text{ g} \times \frac{1 \text{ mol}}{14.01 \text{ g}} = 0.7288 \text{ mol N}$

O: $23.33 \text{ g} \times \frac{1 \text{ mol}}{16.00 \text{ g}} = 1.456 \text{ mol O}$
Solution to Example Empirical Formula Problem

**Step 2:** Calculate the lowest whole-number mole ratio by dividing by the smallest number of moles:

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

So the empirical formula is: \( \text{C}_7\text{H}_7\text{NO}_2 \)
Determining a Molecular Formula: can be done if both the empirical formula and molar mass are known

**Example:** The empirical formula of a compound was found to be CH. The same compound was found to have a molar mass of 78.1 g/mol. What is its molecular formula?

- **First find the (empirical) molar mass based on the empirical formula:**
  
  \[
  \text{Empirical Molar Mass} = 1 \times (12.01) + 1 \times (1.01) = 13.02 \text{ g/emp. mol}
  \]

- **The molecular formula must be a whole-number of the empirical formula. Divide the molar mass by the empirical molar mass to find the whole number:**
  
  \[
  \text{Whole-number multiple} = \frac{78.1 \text{ g/mol}}{13.02 \text{ emp. mol}} = 6.00 = 6
  \]

So the molecular formula is \( \text{C}_6\text{H}_6 \).
More Examples of Empirical and Molecular Mass Problems

Click here to view a video on calculating an empirical formula from mass data.

Click here to view a tutorial video on how to calculate molecular formula of a compound given both its empirical formula and molar mass.

Click here to view a video tutorial on how to calculate both empirical and molecular formulas.
Stoichiometry

- Study of the mass relationships in chemistry
- Based on the **Law of Conservation of Mass** (Antoine Lavoisier, 1789), as explained by the **Atomic Theory of Matter** (John Dalton, 1800)

We may lay it down as an incontestable axiom that, in all the operations of art and nature, nothing is created; an equal amount of matter exists both before and after the experiment. Upon this principle, the whole art of performing chemical experiments depends.

—Antoine Lavoisier
Chemical Equations

- concise representations of chemical reactions.
- based on atomic theory

\[ 2 \text{H}_2 + \text{O}_2 \rightarrow 2 \text{H}_2\text{O} \]
Interpreting a Chemical Equation

Reactants: The Starting Materials

\[ \text{CH}_4(g) + 2\text{O}_2(g) \quad \rightarrow \quad \text{CO}_2(g) + 2\text{H}_2\text{O}(g) \]

Reactants appear on the left side of the equation.
Interpreting a Chemical Equation

Products: New Substances Resulting from a Chemical Change

\[ \text{CH}_4(g) + 2\text{O}_2(g) \rightarrow \text{CO}_2(g) + 2\text{H}_2\text{O}(g) \]

Products appear on the right side of the equation.
Interpreting a Chemical Equation
Physical States of Reactants and Products

\[ \text{CH}_4(g) + 2\text{O}_2(g) \rightarrow \text{CO}_2(g) + 2\text{H}_2\text{O}(g) \]

The *states* of the reactants and products are written in parentheses to the right of each compound.

\( (g) = \text{gas}; (l) = \text{liquid}; (s) = \text{solid}; (aq) = \text{in aqueous solution} \)
Interpreting a Chemical Equation

It Must Be Balanced

\[ \text{CH}_4(g) + 2\text{O}_2(g) \rightarrow \text{CO}_2(g) + 2\text{H}_2\text{O}(g) \]

- **Stoichiometric Coefficients**: used to make the same number of each of atom type appear on each side of the equation, making the equation consistent with the law of conservation of mass.
Don’t Balance by Changing Formula Subscripts:  
**This Changes the Nature of the Reaction**

- Hydrogen and oxygen can make water OR hydrogen peroxide:
  - $\text{2 H}_2(g) + \text{O}_2(g) \rightarrow \text{2 H}_2\text{O}(l)$
  - $\text{H}_2(g) + \text{O}_2(g) \rightarrow \text{H}_2\text{O}_2(l)$

- The above reactions result in two very different products. (Trust me, you don’t want to drink pure $\text{H}_2\text{O}_2$!)
Tutorial Videos:
Writing Balanced Chemical Reactions

Click here to view a tutorial video on how to write unbalanced (skeleton) equations based on written descriptions of chemical reactions.

Click here to view a tutorial video showing how to balance unbalanced skeleton equations for chemical reactions.

Click here for an overview on how to write balanced chemical equations.
Classifying Chemical Reactions

Many reactions fall into one of the following three categories:

- Combination reactions
- Decomposition reactions
- Combustion reactions

Several more reaction classifications will be introduced as the year progresses.
Combination (or Synthesis) Reaction

- Two or more substances react to form one product.
- Some examples:
  \[ \text{N}_2(g) + 3 \text{H}_2(g) \rightarrow 2 \text{NH}_3(g) \]
  \[ \text{C}_3\text{H}_6(g) + \text{Br}_2(l) \rightarrow \text{C}_3\text{H}_6\text{Br}_2(l) \]
  \[ 2 \text{Mg}(s) + \text{O}_2(g) \rightarrow 2 \text{MgO}(s) \]
Decomposition Reaction

- One substance breaks down into two or more substances.
- Some examples:
  
  \[
  \text{CaCO}_3(s) \rightarrow \text{CaO}(s) + \text{CO}_2(g)
  \]
  
  \[
  2 \text{ KClO}_3(s) \rightarrow 2 \text{ KCl}(s) + \text{O}_2(g)
  \]
  
  \[
  2 \text{ NaN}_3(s) \rightarrow 2 \text{ Na}(s) + 3 \text{ N}_2(g) \quad \text{(occurs in car air bags)}
  \]
Combustion Reactions

- Are generally rapid reactions that produce flames.
- Most involve oxygen (from the air) as a reactant.
- Also involve a fuel that reacts with O$_2$ to form one or more oxidized products.
- Complete combustion of hydrocarbon fuels results in the products CO$_2$ and H$_2$O.

- Some examples of hydrocarbon combustion

  \[
  \text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O}(g)
  \]
  \[
  \text{C}_3\text{H}_8(g) + 5 \text{O}_2(g) \rightarrow 3 \text{CO}_2(g) + 4 \text{H}_2\text{O}(g)
  \]
Combustion Analysis

• A common experimental technique used to determine both the compositions (by mass) and empirical formulas of compounds composed of C and H (and sometimes a 3rd element such as O or N).

• Uses an apparatus like that pictured below. A sample of the compound of known mass is combusted, and the products (CO$_2$ and H$_2$O) are collected and massed.

• The next slide gives the general procedure for working up the data from a combustion analysis experiment. It also contains a link to a video tutorial.
Determining an Empirical Formula Based on Combustion Analysis Data

- Given the masses of CO₂ and H₂O produced by combusting a known mass of an unknown hydrocarbon compound. (The compound may also contain one other element, such as O or N).
- All C from the sample is converted to CO₂; so the mass of C in the sample is found from the mass of CO₂ produced (12.01 g C per 44.01 g CO₂).
- All H from the sample is converted to H₂O; so the mass of H in the sample is found from the mass of H₂O produced (2.02 g H per 18.02 g H₂O).
- If needed, the mass of a 3rd element (such as O or N) in the sample is found by subtracting the masses of C and H from the total sample mass.
- The mass data are then used to determine the empirical formula; if the molar mass of the compound is also, one can also determine the molecular formula.

Click here to view a video tutorial on combustion analysis and how it is used to determine chemical formulas. The video gives a quick overview of the combustion analysis technique and then solves a sample problem.
Reaction Stoichiometry:
Quantitative Relationships Between Reactants and Products

**Stoichiometric coefficients** in a balanced equation show:

- relative numbers of atoms/molecules/formula units of reactants and products (submicroscopic point of view).

AND

- relative numbers of *moles* of reactants and products, which can be converted to *mass* (macroscopic level).

![Image of chemical equation: \(2 \text{H}_2(g) + \text{O}_2(g) \rightarrow 2 \text{H}_2\text{O}(l)\) with molecular and mole-level interpretations, and conversion to grams using molar masses resulting in 4.0 g H\(_2\), 32.0 g O\(_2\), and 36.0 g H\(_2\text{O}\).]
Stoichiometric Calculations

- We’ve already seen in this chapter how to convert grams of a substance into moles of the same substance (or moles to grams).
- We’ll now review how to calculate amounts of DIFFERENT substances consumed and/or produced by the same chemical reaction.
- **Stoichiometric Ratio (or “Mole Bridge”):** the “bridge” relating the amounts of two different substances involved in the same reaction. It is obtained from the balanced equation.
**Example:** How many grams of water can be produced from 1.00 g of glucose?

\[ \text{C}_6\text{H}_{12}\text{O}_6(\text{s}) + 6 \text{O}_2(\text{g}) \rightarrow 6 \text{CO}_2(\text{g}) + 6 \text{H}_2\text{O}(\text{l}) \]

**Step 1:** convert the starting amount of 1.00 g of glucose into moles:

\[
\text{Moles C}_6\text{H}_{12}\text{O}_6 = \left(1.00 \text{ g C}_6\text{H}_{12}\text{O}_6\right) \left(\frac{1 \text{ mol C}_6\text{H}_{12}\text{O}_6}{180.0 \text{ g C}_6\text{H}_{12}\text{O}_6}\right)
\]

**Step 2:** convert moles the reactant sucrose into moles of the product water using the appropriate stoichiometric ratio (or “mole bridge”) from the balanced equation:

\[
\text{Moles H}_2\text{O} = \left(1.00 \text{ g C}_6\text{H}_{12}\text{O}_6\right) \left(\frac{1 \text{ mol C}_6\text{H}_{12}\text{O}_6}{180.0 \text{ g C}_6\text{H}_{12}\text{O}_6}\right) \left(\frac{6 \text{ mol H}_2\text{O}}{1 \text{ mol C}_6\text{H}_{12}\text{O}_6}\right)
\]

*Problem continued on next slide.*
**Step 3:** convert moles of the product water to grams of water:

\[
\text{Grams H}_2\text{O} = (1.00 \text{ g C}_6\text{H}_{12}\text{O}_6) \left(\frac{1 \text{ mol C}_6\text{H}_{12}\text{O}_6}{180.0 \text{ g C}_6\text{H}_{12}\text{O}_6}\right) \left(\frac{6 \text{ mol H}_2\text{O}}{1 \text{ mol C}_6\text{H}_{12}\text{O}_6}\right) \left(\frac{18.0 \text{ g H}_2\text{O}}{1 \text{ mol H}_2\text{O}}\right) \\
= 0.600 \text{ g H}_2\text{O}
\]

**Links to some tutorial videos:**

Click here to view a video on how to covert from moles of one substance into moles of another substance using the “mole bridge” from a balanced chemical equation.

Click here to view a video on reaction stoichiometry. This video covers the full process of going from the mass of one substance (reactant or product) in a chemical reaction to the equivalent mass of another substance (reactant or product in the same reaction.)
Limiting Reactant: the reactant present in the smallest “stoichiometric amount” (i.e. the reactant that will run out first).

Example: The following balanced equation shows that in order to form two \( \text{H}_2\text{O} \) molecules, two \( \text{H}_2 \) molecules are required for each \( \text{O}_2 \) molecule.

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

- Starting with 10 \( \text{H}_2 \) molecules and 7 \( \text{O}_2 \) molecules (pictured below), the \( \text{H}_2 \) molecules will run out first (i.e. \( \text{H}_2 \) is the limiting reactant).
- A maximum of ten \( \text{H}_2\text{O} \) molecules can form before the \( \text{H}_2 \) runs out, leaving two \( \text{O}_2 \) unused molecules (i.e. \( \text{O}_2 \) is the excess reactant).
Theoretical and Actual Yields

**Theoretical yield**: maximum amount of product that can be made (before the limiting reactant runs out).

- e.g. On the previous slide, the theoretical yield is 10 H$_2$O molecules.
- A theoretical yield calculation must be performed whenever definite amounts of more than one reactant are given.

**Actual yield**: amount of product that is actually measured. It is often different from the theoretical yield:

- Percent-Yield = (Actual Yield) / (Theoretical Yield) × 100%
- %-yield can be less than 100% if, among other reasons, the reaction achieves equilibrium before coming to completion or if some reactants and/or products are physically lost going from one experimental step to another.
- %-yield can be greater than 100% if the product contains impurities. These may include left-over reactants and/or undesired by-products that were not successfully separated from the desired product.
Tutorial Videos on Calculating Limiting Reactants, Theoretical Yields, and Percent Yields

Click here for a tutorial on the concept of theoretical yield, including some sample calculations. Note: theoretical yields are also calculated; however the term is never used explicitly.

Click here to view a tutorial on calculating the amount of excess reactant remaining after a reaction is 100% complete. Limiting reactant and theoretical yield calculations are also included.

Click here to view the solution to a simple percent-yield problem. The video also reviews the concepts of theoretical yield and actual yield.

Click here to view the solution to a combined limiting reactant & percent yield problem.