Chapter 3
Stoichiometry: Calculations with Chemical Formulas and Equations
Anatomy of a Chemical Equation

\[ CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g) \]
Anatomy of a Chemical Equation

**Reactants** appear on the left side of the equation.

\[
\text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O}(g)
\]
Anatomy of a Chemical Equation

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

Products appear on the right side of the equation.
The states of the reactants and products are written in parentheses to the right of each compound.
Anatomy of a Chemical Equation

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

Coefficients are inserted to balance the equation.
Subscripts and Coefficients Give Different Information

<table>
<thead>
<tr>
<th>Chemical symbol</th>
<th>Meaning</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>One molecule of water:</td>
<td>Two H atoms and one O atom</td>
</tr>
<tr>
<td>$2 \text{H}_2\text{O}$</td>
<td>Two molecules of water:</td>
<td>Four H atoms and two O atoms</td>
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- Subscripts tell the number of atoms of each element in a molecule
### Subscripts and Coefficients Give Different Information

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<td>Two molecules of water:</td>
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</table>

- Subscripts tell the number of atoms of each element in a molecule.
- Coefficients tell the number of molecules (compounds).
Reaction Types
Combination Reactions

• Two or more substances react to form one product

Examples:

\[ \text{N}_2 (g) + 3 \text{H}_2 (g) \rightarrow 2 \text{NH}_3 (g) \]
\[ \text{C}_3\text{H}_6 (g) + \text{Br}_2 (l) \rightarrow \text{C}_3\text{H}_6\text{Br}_2 (l) \]
\[ 2 \text{Mg} (s) + \text{O}_2 (g) \rightarrow 2 \text{MgO} (s) \]
2 Mg\textsubscript{(s)} + O\textsubscript{2}\textsubscript{(g)} \rightarrow 2 \text{MgO\textsubscript{(s)}}
Decomposition Reactions

- One substance breaks down into two or more substances

Examples:

\[ \text{CaCO}_3 (s) \rightarrow \text{CaO} (s) + \text{CO}_2 (g) \]
\[ 2 \text{KClO}_3 (s) \rightarrow 2 \text{KCl} (s) + \text{O}_2 (g) \]
\[ 2 \text{NaN}_3 (s) \rightarrow 2 \text{Na} (s) + 3 \text{N}_2 (g) \]
Combustion Reactions

- Rapid reactions that have oxygen as a reactant sometimes produce a flame
- Most often involve hydrocarbons reacting with oxygen in the air to produce CO$_2$ and H$_2$O.

**Examples:**

\[
\begin{align*}
\text{CH}_4 (g) + 2 \text{ O}_2 (g) & \rightarrow \text{ CO}_2 (g) + 2 \text{ H}_2\text{O} (g) \\
\text{C}_3\text{H}_8 (g) + 5 \text{ O}_2 (g) & \rightarrow 3 \text{ CO}_2 (g) + 4 \text{ H}_2\text{O} (g)
\end{align*}
\]
Formula Weights
Formula Weight (FW)

- Sum of the atomic weights for the atoms in a chemical formula
- So, the formula weight of calcium chloride, CaCl$_2$, would be
  \[
  \text{Ca: } 1(40.1 \text{ amu}) \\
  + \text{Cl: } 2(35.5 \text{ amu}) \\
  \quad 111.1 \text{ amu}
  \]
- These 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

\[
\begin{align*}
\text{C:} & \quad 2(12.0 \text{ amu}) \\
\text{+ H:} & \quad 6(1.0 \text{ amu}) \\
\hline
30.0 \text{ amu}
\end{align*}
\]
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:

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

So the percentage of carbon and hydrogen in ethane ($\text{C}_2\text{H}_6$, molecular mass = 30.0) is:

$$%\text{C} = \frac{(2)(12.0 \text{ amu})}{(30.0 \text{ amu})} = \frac{24.0 \text{ amu}}{30.0 \text{ amu}} \times 100 = 80.0\%$$

$$%\text{H} = \frac{(6)(1.01 \text{ amu})}{(30.0 \text{ amu})} = \frac{6.06 \text{ amu}}{30.0 \text{ amu}} \times 100 = 20.0\%$$
Moles
Atomic mass unit and the mole

- amu definition: $^{12}\text{C} = 12$ amu.
- The atomic mass unit is defined this way.
- How many $^{12}\text{C}$ atoms weigh 12 g?
  - $6.02 \times 10^{23}^{12}\text{C}$ weigh 12 g.
- Avagadro’s number
- The mole
Therefore:

- $6.02 \times 10^{23}$
- 1 mole of $^{12}$C has a mass of 12 g

Stoichiometry
The mole

- The mole is just a number of things
- 1 dozen = 12 things
- 1 pair = 2 things
- 1 mole = $6.02 \times 10^{23}$ things
Molar Mass

The trick:

• By definition, these are the mass of 1 mol of a substance (i.e., g/mol)
  – The molar mass of an element is the mass number for the element that we find on the periodic table
  – The formula weight (in amu’s) will be the same number as the molar mass (in g/mol)
Moles provide a bridge from the molecular scale to the real-world scale.

The number of moles correspond to the number of molecules. 1 mole of any substance has the same number of molecules.
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>6.022 \times 10^{23} N atoms</td>
</tr>
<tr>
<td>Molecular nitrogen</td>
<td>N\textsubscript{2}</td>
<td>28.0</td>
<td>28.0</td>
<td>6.022 \times 10^{23} N\textsubscript{2} molecules</td>
</tr>
<tr>
<td>Silver</td>
<td>Ag</td>
<td>107.9</td>
<td>107.9</td>
<td>6.022 \times 10^{23} Ag atoms</td>
</tr>
<tr>
<td>Silver ions</td>
<td>Ag\textsuperscript{+}</td>
<td>107.9\textsuperscript{a}</td>
<td>107.9</td>
<td>6.022 \times 10^{23} Ag\textsuperscript{+} ions</td>
</tr>
<tr>
<td>Barium chloride</td>
<td>BaCl\textsubscript{2}</td>
<td>208.2</td>
<td>208.2</td>
<td>6.022 \times 10^{23} BaCl\textsubscript{2} units</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>6.022 \times 10^{23} Ba\textsuperscript{2+} ions</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2(6.022 \times 10^{23}) Cl\textsuperscript{−} ions</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Recall that the electron has negligible mass; thus, ions and atoms have essentially the same mass.

- One mole of atoms, ions, or molecules contains Avogadro’s number of those particles
- One mole of molecules or formula units contains Avogadro’s number times the number of atoms or ions of each element in the compound
Finding Empirical Formulas
Calculating Empirical Formulas

One can calculate the empirical formula from the percent composition.
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.
Calculating Empirical Formulas

Assuming 100.00 g of *para*-aminobenzoic acid,

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

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

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

These are the subscripts for the empirical formula:

\[ \text{C}_7\text{H}_7\text{NO}_2 \]
Compounds containing C, H and O are routinely analyzed through combustion in a chamber like this:

- C is determined from the mass of CO$_2$ produced
- H is determined from the mass of H$_2$O produced
- O is determined by difference after the C and H have been determined
Elemental Analyses

Compounds containing other elements are analyzed using methods analogous to those used for C, H and O
**Stoichiometric Calculations**

<table>
<thead>
<tr>
<th>Equation:</th>
<th>2 $\text{H}_2(g)$ + $\text{O}_2(g)$ $\rightarrow$ 2 $\text{H}_2\text{O}(l)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecules:</td>
<td>2 molecules $\text{H}_2$ + 1 molecule $\text{O}_2$ $\rightarrow$ 2 molecules $\text{H}_2\text{O}$</td>
</tr>
<tr>
<td>Mass (amu):</td>
<td>4.0 amu $\text{H}_2$ + 32.0 amu $\text{O}_2$ $\rightarrow$ 36.0 amu $\text{H}_2\text{O}$</td>
</tr>
<tr>
<td>Amount (mol):</td>
<td>2 mol $\text{H}_2$ + 1 mol $\text{O}_2$ $\rightarrow$ 2 mol $\text{H}_2\text{O}$</td>
</tr>
<tr>
<td>Mass (g):</td>
<td>4.0 g $\text{H}_2$ + 32.0 g $\text{O}_2$ $\rightarrow$ 36.0 g $\text{H}_2\text{O}$</td>
</tr>
</tbody>
</table>

The coefficients in the balanced equation give the ratio of *moles* of reactants and products.
Stoichiometric Calculations

From the mass of Substance A you can use the ratio of the coefficients of A and B to calculate the mass of Substance B formed (if it’s a product) or used (if it’s a reactant)
Stoichiometric Calculations

\[ C_6H_{12}O_6 + 6 O_2 \rightarrow 6 CO_2 + 6 H_2O \]

Starting with 10. g of \( C_6H_{12}O_6 \)...
we calculate the moles of \( C_6H_{12}O_6 \)...
use the coefficients to find the moles of \( H_2O \) & \( CO_2 \)
and then turn the moles to grams
Stoichiometric calculations

\[ \text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \rightarrow 6\text{CO}_2 + 6\text{H}_2\text{O} \]

- Mass: 10.0 g
- MW: 180 g/mol
- Mol: 10.0 g \times \frac{1 \text{ mol}}{180 \text{ g}} = 0.055 \text{ mol}
- MW of \text{CO}_2 = 44 \text{ g/mol}
- MW of \text{H}_2\text{O} = 18 \text{ g/mol}
- Grams of \text{CO}_2 = 0.055 \text{ mol} \times 44 \text{ g/mol} = 2.38 \text{ g}
- Grams of \text{H}_2\text{O} = 0.055 \text{ mol} \times 18 \text{ g/mol} = 0.99 \text{ g}

Total:
- Grams: 2.38 g + 0.99 g = 3.37 g
- Mol: 0.055 mol
Limiting Reactants
How Many Cookies Can I Make?

- You can make cookies until you run out of one of the ingredients.
- Once you run out of sugar, you will stop making cookies (at least any cookies you would want to eat).
How Many Cookies Can I Make?

- In this example the sugar would be the limiting reactant, because it will limit the amount of cookies you can make.
Limiting Reactants

- The limiting reactant is the reactant present in the smallest stoichiometric amount

\[ 2H_2 + O_2 \rightarrow 2H_2O \]

<table>
<thead>
<tr>
<th>#moles</th>
<th>14</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10</td>
<td>5</td>
</tr>
<tr>
<td>Left:</td>
<td>0</td>
<td>2</td>
</tr>
</tbody>
</table>

10 \( H_2 \) and 7 \( O_2 \) | 10 \( H_2O \) and 2 \( O_2 \)
Limiting Reactants

In the example below, the $\text{O}_2$ would be the excess reagent

Before reaction

10 $\text{H}_2$ and 7 $\text{O}_2$

After reaction

10 $\text{H}_2\text{O}$ and 2 $\text{O}_2$
Limiting reagent, example:

Soda fizz comes from sodium bicarbonate and citric acid \( (\text{H}_3\text{C}_6\text{H}_5\text{O}_7) \) reacting to make carbon dioxide, sodium citrate \( (\text{Na}_3\text{C}_6\text{H}_5\text{O}_7) \) and water. If 1.0 g of sodium bicarbonate and 1.0g citric acid are reacted, which is limiting? How much carbon dioxide is produced?

\[
3\text{NaHCO}_3(aq) + \text{H}_3\text{C}_6\text{H}_5\text{O}_7(aq) \rightarrow 3\text{CO}_2(g) + 3\text{H}_2\text{O}(l) + \text{Na}_3\text{C}_6\text{H}_5\text{O}_7(aq)
\]

1.0g \hspace{1cm} 1.0g

84g/mol \hspace{1cm} 192g/mol \hspace{1cm} 44g/mol

1.0g(1mol/84g) \hspace{1cm} 1.0(1mol/192g)

0.012 mol \hspace{1cm} 0.0052 mol

0.0052(3)=0.016 \hspace{1cm} 0.0052 mol

(If citrate limiting)

0.012 mol \hspace{1cm} 0.012(1/3)=.0040mol \hspace{1cm} 0.012 moles \text{CO}_2

44g/mol(0.012mol)=0.53g \text{CO}_2

.0052-.0040=.0012 \text{ left}

0.0012mol(192g/mol)=

0.023 \text{ g left.}
Theoretical Yield

• The theoretical yield is the amount of product that can be made
  – In other words it’s the amount of product possible from stoichiometry. The “perfect reaction.”

• This is different from the actual yield, the amount one actually produces and measures
Percent Yield

A comparison of the amount actually obtained to the amount it was possible to make

\[
\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100
\]
Example

Benzene (C₆H₆) reacts with Bromine to produce bromobenzene and hydrobromic acid. If 30. g of benzene reacts with 65 g of bromine and produces 56.7 g of bromobenzene, what is the percent yield of the reaction?

\[
\text{C}_6\text{H}_6 + \text{Br}_2 \rightarrow \text{C}_6\text{H}_5\text{Br} + \text{HBr}
\]

<table>
<thead>
<tr>
<th>C₆H₆</th>
<th>+</th>
<th>Br₂</th>
<th>-----&gt;</th>
<th>C₆H₅Br</th>
<th>+</th>
<th>HBr</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.g</td>
<td></td>
<td>65 g</td>
<td></td>
<td>?</td>
<td></td>
<td>?</td>
</tr>
<tr>
<td>78g/mol</td>
<td></td>
<td>160.g/mol</td>
<td></td>
<td>157g/mol</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30.g(1mol/78g)</td>
<td></td>
<td>65g(1mol/160g)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.38 mol</td>
<td></td>
<td>0.41 mol</td>
<td></td>
<td>0.38 mol</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

0.38mol(157g/1mol)
60.g
57g/60.g(100)=95%
Example, one more

React 1.5 g of NH$_3$ with 2.75 g of O$_2$. How much NO and H$_2$O is produced? What is left?

\[
\begin{align*}
4\text{NH}_3 & \quad + \quad 5\text{O}_2 \quad \longrightarrow \quad 4\text{NO} \quad + \quad 6\text{H}_2\text{O} \\
1.5\text{g} & \quad 2.75\text{g} & \quad ? & \quad ? \\
17\text{g/mol} & \quad 32\text{g/mol} & \quad 30.\text{g/mol} & \quad 18\text{g/mol} \\
1.5\text{g}(1\text{mol/17g}) & \quad 2.75\text{g}(1\text{mol/32g}) & \quad .088\text{mol} & \quad .086 \\
.088\text{mol} & \quad .086 & \quad .086(4/5) & \quad 11 \\
.086(4/5) & \quad .086\text{mol} & \quad .086\text{mol}(4/5) & \quad .086(6/5) \\
.069\text{mol} & \quad .069\text{mol} & \quad .069\text{mol}(30.\text{g/mol}) & \quad .10\text{mol} \\
.069\text{mol}(17\text{g/mol}) & \quad .069\text{mol} & \quad .069\text{mol}(18\text{g/mol}) & \quad .10\text{mol}(18\text{g/mol}) \\
1.2\text{g} & \quad 2.75\text{g} & \quad 2.1\text{g} & \quad 1.8\text{g}
\end{align*}
\]