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

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

Reactants appear on the left side of the equation.

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

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

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

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>
</tr>
<tr>
<td>$\text{H}_2\text{O}_2$</td>
<td>One molecule of hydrogen peroxide:</td>
<td>Two H atoms and two O atoms</td>
</tr>
</tbody>
</table>

- Subscripts tell the number of atoms of each element in a molecule
Subscripts and Coefficients Give Different Information

- Subscripts tell the number of atoms of each element in a molecule or compound.
- Coefficients tell the number of molecules or entities (compounds).

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<tr>
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</tr>
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<tbody>
<tr>
<td>H₂O</td>
<td>One molecule of water:</td>
<td>Two H atoms and one O atom</td>
</tr>
<tr>
<td>2 H₂O</td>
<td>Two molecules of water:</td>
<td>Four H atoms and two O atoms</td>
</tr>
<tr>
<td>H₂O₂</td>
<td>One molecule of hydrogen peroxide:</td>
<td>Two H atoms and two O atoms</td>
</tr>
</tbody>
</table>

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Reaction Types.
Combination Reactions

• Two or more substances react to form one product

Example:

\[
\text{N}_2 (g) + 3 \text{H}_2 (g) \rightarrow 2 \text{NH}_3 (g)
\]

\[
\text{C}_3\text{H}_6 (g) + \text{Br}_2 (l) \rightarrow \text{C}_3\text{H}_6\text{Br}_2 (l)
\]

\[
2 \text{Mg} (s) + \text{O}_2 (g) \rightarrow 2 \text{MgO} (s)
\]
Decomposition Reactions
One reactant decomposes to more than one or more products

• One substance breaks down into two or more substances

• Examples:

  CaCO$_3$ (s) $\rightarrow$ CaO (s) + CO$_2$ (g)
  2 KClO$_3$ (s) $\rightarrow$ 2 KCl (s) + O$_2$ (g)
  2 NaN$_3$ (s) $\rightarrow$ 2 Na (s) + 3 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:

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

- Defined (since 1961) as:
  - 1/12 mass of the $^{12}\text{C}$ isotope.
  - $^{12}\text{C} = 12$ amu
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
  
  \[
  \text{Ca: } 1(40.1 \text{ amu}) \\
  \text{ + Cl: } 2(35.5 \text{ amu}) \\
  \text{111.1 amu}
  \]

- 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

$$\text{C: } 2(12.0 \text{ amu}) + \text{H: } 6(1.0 \text{ amu}) = 30.0 \text{ amu}$$
Percent Composition

The percent composition by element:

\[
\% \text{ element} = \frac{\text{(# of atoms of element)} \times \text{(atomic weight)}}{\text{(FW of the compound)}} \times 100
\]
So the percentage of carbon and hydrogen in ethane (C$_2$H$_6$, molecular mass = 30.0) is:

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

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

- amu definition: $^{12}\text{C} = 12$ amu.
- The atomic mass unit is defined this way.
- $1$ amu = $1.6605 \times 10^{-24}$ g
- How many $^{12}\text{C}$ atoms weigh $12$ g?
- $6.02221409 \times 10^{23}^{12}\text{C}$ weigh $12$ g.
- Avogadro’s number
- *The mole*
Atomic mass unit and the mole

- amu definition: $^{12}\text{C} = 12 \text{ amu}$.
- $1 \text{ amu} = 1.6605 \times 10^{-24} \text{ g}$
- How many $^{12}\text{C}$ atoms weigh 12 g?
- $6.0221409 \times 10^{23} ^{12}\text{C}$ weigh 12 g.
- Avogadro’s number
- The mole

- $\# \text{atoms} = (1 \text{ atom} / 12 \text{ amu}) (1 \text{ amu} / 1.66 \times 10^{-24} \text{ g}) (12 \text{ g})$
  $= 6.02 \times 10^{23} ^{12}\text{C} \text{ weigh 12 g}$
Therefore:

- $6.02 \times 10^{23}$
- 1 mole of $^{12}\text{C}$ has a mass of 12 g
- 1 mole of $\text{H}_2\text{O}$ has a mass of 18.0 g!
The mole

- The mole is just a number of things
- 1 dozen = 12 things
- 1 pair = 2 things
- 1 mole = $6.022141 \times 10^{23}$ things
- $6.022141 \times 10^{23}$ atoms/mole
- SO
- 1 mole C atoms = $6.022 \times 10^{23}$ C atoms
Molar Mass

The trick:

• By definition, this is 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

- 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.

<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 { 6.022 \times 10^{23} N_2 molecules, 2(6.022 \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>{ 6.022 \times 10^{23} N_2 molecules, 2(6.022 \times 10^{23}) N atoms }</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 { 6.022 \times 10^{23} Ag^+ ions, 6.022 \times 10^{23} BaCl_2 units }</td>
</tr>
<tr>
<td>Silver ions</td>
<td>Ag^+</td>
<td>107.9^a</td>
<td>107.9</td>
<td>{ 6.022 \times 10^{23} Ag^+ ions, 6.022 \times 10^{23} Ba^{2+} ions }</td>
</tr>
<tr>
<td>Barium chloride</td>
<td>BaCl_2</td>
<td>208.2</td>
<td>208.2</td>
<td>2(6.022 \times 10^{23}) Cl^- ions { 6.022 \times 10^{23} BaCl_2 units }</td>
</tr>
</tbody>
</table>

^aRecall that the electron has negligible mass; thus, ions and atoms have essentially the same mass.
Finding Empirical Formulas
Combustion Analysis gives % composition

Compounds containing C, H and O are routinely analyzed through combustion in a chamber like this:

- %C is determined from the mass of CO\textsubscript{2} produced
- %H is determined from the mass of H\textsubscript{2}O produced
- %O is determined by difference after the C and H have been determined

\[ \text{C}_n\text{H}_n\text{O}_n + \text{O}_2 \rightarrow n\text{CO}_2 + \frac{1}{2}n\text{H}_2\text{O} \]
Calculating Empirical Formulas

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

The compound \textit{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

1. Assuming 100.00 g of *para*-aminobenzoic acid, find out how many moles of each element are in that 100 g:

   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: \[ 23.33 \text{ g} \times \frac{1 \text{ mol}}{16.00 \text{ g}} = 1.456 \text{ mol O} \]
Calculating Empirical Formulas

2. Calculate the mole ratio by dividing moles of each element by the number of moles of the element with the least number of moles:

- **C:** \[rac{5.105 \text{ mol}}{0.7288 \text{ mol}} = 7.005 \approx 7 \]
- **H:** \[rac{5.09 \text{ mol}}{0.7288 \text{ mol}} = 6.984 \approx 7 \]
- **N:** \[rac{0.7288 \text{ mol}}{0.7288 \text{ mol}} = 1.000 \]
- **O:** \[rac{1.458 \text{ mol}}{0.7288 \text{ mol}} = 2.001 \approx 2 \]
Calculating Empirical Formulas

These are the subscripts for the empirical formula:

\[ \text{C}_7\text{H}_7\text{NO}_2 \]
Elemental Analyses

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

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

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

Example: 10 grams of glucose (C₆H₁₂O₆) react in a combustion reaction. How many grams of each product are produced?

C₆H₁₂O₆(s) + 6 O₂(g) → 6 CO₂(g) + 6 H₂O(l)

10. g → ? + ?

Starting with 10. g of C₆H₁₂O₆...
we calculate the moles of C₆H₁₂O₆...
use the coefficients to find the moles of H₂O & CO₂
and then turn the moles to grams
Stoichiometric calculations

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

10.0 g                                ?          +                 ?

MW: 180 g/mol                                    44 g/mol                             18 g/mol

#mol: 10.0 g (1 mol/180 g)

0.055 mol                          6(0.055)                          6(0.055 mol)

6(0.055 mol) 44 g/mol        6(0.055 mol) 18 g/mol

#grams:                          15 g                                 5.9 g

How many grams of oxygen reacted?
Stoichiometric calculations

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

10.0 g 
MW: 180 g/mol 
#mol: 10.0 g (1 mol / 180 g)

0.055 mol 
6 (0.055) 
6 (0.055 mol) 44 g/mol 
6 (0.055 mol) 18 g/mol 

#grams: 
15 g 
5.9 g

How many grams of oxygen reacted? 
15 + 5.9 - 10 = 10.9 g
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
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.

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

<table>
<thead>
<tr>
<th>Reactant</th>
<th>Before Reaction</th>
<th>After Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\text{H}_2)</td>
<td>10</td>
<td>0</td>
</tr>
<tr>
<td>(\text{O}_2)</td>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>(\text{H}_2\text{O})</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>
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 1.0 g citric acid are reacted, which is limiting? How much carbon dioxide is produced?

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

1.0g 1.0g
84g/mol 192g/mol 44g/mol
1.0g(1mol/84g) 1.0g(1mol/192g)
0.012 mol 0.0052 mol

(if citrate limiting)

0.0052(3)=0.016 moles bicarbonate, but only have 0.012 moles

So bicarbonate limiting:

0.012 mol 0.012(1/3)=.0040mol 0.012 moles \( \text{CO}_2 \)
44g/mol(0.012mol)=0.53g \( \text{CO}_2 \)

.0052-.0040=.0012mol left
0.0012 mol(192 g/mol)= 0.23 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 (C₆H₅Br) 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>Mass</th>
<th>Molar Mass</th>
<th>Mol. Calculated</th>
</tr>
</thead>
<tbody>
<tr>
<td>30. g</td>
<td>78 g/mol</td>
<td>0.38 mol</td>
</tr>
<tr>
<td>65 g</td>
<td>160 g/mol</td>
<td>0.41 mol</td>
</tr>
<tr>
<td>56.7 g</td>
<td>157 g/mol</td>
<td></td>
</tr>
</tbody>
</table>

\[
(\text{If Br}_2 \text{ limiting})\\
0.41 \text{ mol} + 0.41 \text{ mol}
\]

\[
(\text{If C}_6\text{H}_6 \text{ limiting})\\
0.38 \text{ mol} + 0.38 \text{ mol}
\]

\[
0.38 \text{ mol}(157 \text{ g/mol}) = 60 \text{ g}\\
56.7 \text{ g}/60 \text{ g}(\text{100}) = 94.5\%\approx 95\%
\]
React 1.5 g of NH₃ with 2.75 g of O₂. How much NO and H₂O is produced? What is left?

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

\[
\begin{array}{cccc}
\text{NH}_3 & \text{O}_2 & \text{NO} & \text{H}_2\text{O} \\
1.5\text{g} & 2.75\text{g} & ? & ? \\
17\text{g/mol} & 32\text{g/mol} & 30.\text{g/mol} & 18\text{g/mol} \\
\end{array}
\]

\[
\begin{array}{cccc}
1.5\text{g}(1\text{mol}/17\text{g}) & = & 0.088\text{mol} \\
2.75\text{g}(1\text{mol}/32\text{g}) & = & 0.086\text{mol} \\
(\text{If NH}_3 \text{ limiting}) & & 0.088(5/4) = 11 \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{O}_2 \text{ limiting}: \\
0.086(4/5) & = & 0.086\text{ mol} \\
0.069\text{mol} & & 0.086(4/5) = 0.069\text{ mol} \\
0.069\text{mol}(17\text{g/mol}) & & 0.069\text{mol}(30.\text{g/mol}) \\
1.2\text{g} & = & 2.75\text{g} \\
1.5 \text{ g} - 1.2 \text{ g} = .3\text{g} \\
\end{array}
\]
2HNO$_3$ + 2Cu -----> NO + NO$_2$ + 2Cu$^{2+}$ + 2H$^+$

3 NO + CS$_2$ -> 3/2 N$_2$ + CO + SO$_2$ + 1/8 S$_8$

4 NO + CS$_2$ -> 2 N$_2$ + CO$_2$ + SO$_2$ + 1/8 S$_8$
Gun powder reaction

• $10\text{KNO}_3(s) + 3\text{S}_3(s) + 8\text{C}_3(s) \rightarrow 2\text{K}_2\text{CO}_3(s) + 3\text{K}_2\text{SO}_4(s) + 6\text{CO}_2(g) + 5\text{N}_2(g)$

• Salt peter  sulfur  charcoal

And heat.

What is interesting about this reaction?
What kind of reaction is it?
What do you think makes it so powerful?
Gun powder reaction

- Oxidizing agent: $10\text{KNO}_3(s)$
- Oxidizing agent: $3\text{S}_3(s)$
- Reducing agent: $8\text{C}_3(s)$
- Oxidizing agent: $2\text{K}_2\text{CO}_3(s)$
- Oxidizing agent: $3\text{K}_2\text{SO}_4(s)$
- Reducing agent: $6\text{CO}_2(g)$
- Reducing agent: $5\text{N}_2(g)$

Salt peter, sulfur, charcoal

And heat.

What is interesting about this reaction?
Lots of energy, no oxygen
What kind of reaction is it?
Oxidation reduction
What do you think makes it so powerful and explosive?
Makes a lot of gas!!!!
White phosphorous and Oxygen under water
$2 \text{Mg}_{(s)} + \text{O}_2_{(g)} \rightarrow 2 \text{MgO}_{(s)}$