CHAPTER 3

Chemical Reactions

Quantities of Reactants and Products

"Stoichiometry"

Application of
The Law of Conservation of Matter

Chemical book-keeping

Chemical Equations

- Chemical equations:
  - Describe proportions of **reactants** (the substances that are consumed) and **products** (the substances that are formed) during a chemical reaction.
  - Describe the changes on the atomic level.
    - » $SO_3(g) + H_2O(l) \rightarrow H_2SO_4(l)$
    - » $Fe_2O_3(s) + 3H_2SO_4(aq) \rightarrow 3H_2O(l) + Fe_2(SO_4)_3(aq)$
  - Physical state of products/reactants:
    - » (*s*) = solid; (*l*) = liquid; (*g*) = gas; (*aq*) = aqueous soln.

Chemical Reactions

Combination Reaction: two or more substances combine to form one product.

$$SO_3(g) + H_2O(g) \rightarrow H_2SO_4(l)$$

A chemical reaction will *change the arrangements* of atoms in substances; but it *neither destroy nor create atoms* (matter) because of the reaction.

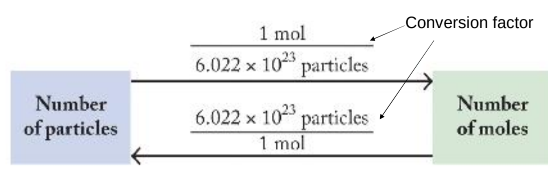
The quantitative nature of chemical reactions arises from the law of conservation of matter.

The Mole: 'Amounts' in Chemistry are expressed in the unit of mole(s).

- A "mole" is a unit for a specific number:
  - 1 dozen = 12 items
  - 1 mole = 6.022×10^{23} particles (molecules/atoms) (also known as Avogadro's number)
- A mole is the Avogadro's number of atoms in exactly 12 grams of carbon-12 isotope.
- Mole - convenient unit for expressing macroscopic quantities (atoms or molecules) involved in chemical reactions.

Mole as Conversion Factor:

- To convert between number of particles and an equivalent number of moles:
  - Divide or multiply by Avogadro's number



Molar Mass:

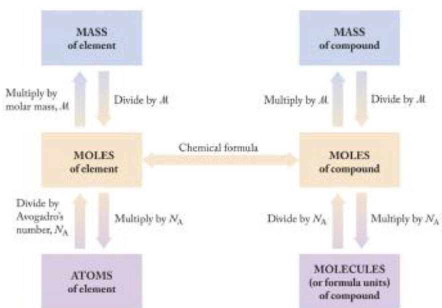
- Molar mass:
  - The molecular mass is the mass of an individual (atom, formula unit or) molecule (in amu).
  - Molar mass is the mass (in grams) of one mole of the substance (atoms, molecules, or formula units ← ionic compounds):
    - » 1 atom of He = 4.003 amu
    - » 1 mole of He (i.e.6.022 × 10^{23} atoms) = 4.003 g
  - The molar mass ($\mathcal{M}$) of He 4.003 g/mol.

Molar Mass of Compounds:

- The mass (in grams) of one mole of the compound.
- Sum of masses of atoms in chemical formula:

$$CO_2 = C + 2\,O$$
$$= 12.01 + 2(16.00)$$
$$= 44.01 g/mol$$

Conversions: Atoms/Molecules to Moles to Mass



Practice: Mole Calculations

Atoms ↔ Moles

a) How many moles of Ca atoms are present in 20.0 g of calcium?

b) How many molecules are present in 5.32 g of chalk ($CaCO_3$)?

Practice: Mole Calculations

Moles ↔ Grams

a) How many grams are present in 3.40 moles of nitrogen gas (N_2)?

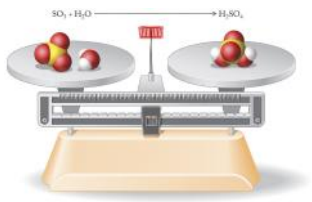
b) How many moles are present in 58.4 g of chalk ($CaCO_3$)?

Practice: Mole Calculations

The uranium used in nuclear fuel exists in nature in several minerals. Calculate how many moles of uranium are found in 100.0 grams of carnotite of molecular formula, $K_2(UO_2)_2(VO_4)_2{\cdot}3H_2O$.

Law of Conservation of Mass

The law of conservation of mass states that the sum of the masses of the reactants of a chemical equation is equal to the sum of the masses of the products.



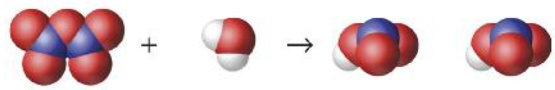
Stoichiometry

- Relationship between the number of moles of reactants and products needed for the conservation of mass.
- Indicated in chemical equation by stoichiometric coefficients.
  - » $Fe_2O_3(s) + 3H_2SO_4(aq) \rightarrow 3H_2O(l) + Fe_2(SO_4)_3(aq)$

Chemical Change

- Chemical reactions follow the law of conservation of mass (balanced chemical reactions)

$$N_2O_5(g) \; + \; H_2O(g) \rightarrow \; 2\,HNO_3(\ell)$$



Balanced Chemical Equations

- Balanced chemical equations follow the law of conservation of mass.
  - Total mass/moles of each element on the reactant side must equal the total mass/moles of each element on the product side.
  - Total charge of reactant side must equal the total charge of product side.

Balancing chemical reactions (coefficients?):

(all chemical formulae must be known)

1. Write the skeletal equation
2. Look for element appearing the least number of times on both sides.
3. Balance that element
4. Check for overall balance
5. Repeat 2 thro' 4 for all elements, if necessary.
6. (later)

Dinitrogen pentoxide gas reacts with water to form nitric acid solution. Write the balanced equation.

Example: $N_2O_5(g) + H_2O(g) \rightarrow HNO_3(l)$

1. *Write correct formulas* (see above) - skeletal equation
2. *Balance element that appearing least in reactant and or product.*

$$N_2O_5(g) + H_2O(g) \rightarrow 2HNO_3(l)$$

$$MnO_2 + KOH + O_2 \rightarrow K_2MnO_4 + H_2O$$

$MnO_2 + 2KOH + O_2 \rightarrow K_2MnO_4 + H_2O$

balancing K did not affect Mn.

H already balanced.

O next

$MnO_2 + 2KOH + O_2 \rightarrow K_2MnO_4 + H_2O$

6 O 5 O

$MnO_2 + 2KOH + \frac{1}{2}O_2 \rightarrow K_2MnO_4 + H_2O$

$MnO_2 + 2KOH + \frac{1}{2}O_2 \rightarrow K_2MnO_4 + H_2O$

Do not leave fractions as coefficients.

$2MnO_2 + 4KOH + O_2 \rightarrow 2K_2MnO_4 + 2H_2O$

$NO_2 + H_2O \rightarrow HNO_3 + NO$

No element is balanced.

first balance H (appears only once)

$NO_2 + H_2O \rightarrow 2HNO_3 + NO$

next N

1N 3N

$3NO_2 + H_2O \rightarrow 2HNO_3 + NO$

balancing all elements but *one*, automatically balances that '*one*'.

6. When one/more polyatomic ions are present, treat them as a single entity.

Ex.

$Na_3PO_4 + Ba(NO_3)_2 \rightarrow Ba_3(PO_4)_2 + NaNO_3$

$Na_3PO_4 + Ba(NO_3)_2 \rightarrow Ba_3(PO_4)_2 + NaNO_3$

$Na_3PO_4 + Ba(NO_3)_2 \rightarrow Ba_3(PO_4)_2 + 3NaNO_3$

$Na_3PO_4 + 3Ba(NO_3)_2 \rightarrow Ba_3(PO_4)_2 + 3NaNO_3$

$2Na_3PO_4 + 3Ba(NO_3)_2 \rightarrow Ba_3(PO_4)_2 + 3NaNO_3$

$2Na_3PO_4 + 3Ba(NO_3)_2 \rightarrow Ba_3(PO_4)_2 + 6NaNO_3$

Hydrogen peroxide, H_2O_2, is a powerful multipurpose reagent and reacts with potassium permanganate (permanganate MnO_4^{-1}) and sulfuric acid H_2SO_4 to produce potassium sulfate, manganese (II) sulfate, water and oxygen.

Write the balanced chemical reaction of the process described above.

Balanced equation - viewed in many ways.

$Fe_2O_3(s) + 3H_2SO_4(aq) \rightarrow 3H_2O(l) + Fe_2(SO_4)_3(aq)$

1 molecule	3 molecules	3 molecules	1 molecule
1 mol	3 mol	3 mol	1 mol
159.69g	3×98.08g	3×18.02g	399.88g
y mol	3y mol	3y mol	y mol
y × 159.69g	y × 294.24g	y × 54.06g	y × 399.88g

Combustion Reactions

- Reactions between oxygen (O_2) and another element in a compound.
  - $4SO_2(g) + 2O_2(g) \rightarrow 4SO_3(g)$
- Hydrocarbons:
  - Molecular compounds composed of only hydrogen and carbon.
  - "Organic" compounds.
  - Combustion products are CO_2 and H_2O.

$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$

Practice: Combustion Reactions

Balance the following equations for the following combustion reactions:

a) $CH_4(g) + O_2(g) \rightarrow CO_2(g) + H_2O(g)$

b) $C_3H_8 + O_2 \rightarrow CO_2 + H_2O$

c) $C_5H_{10} + O_2 \rightarrow CO_2 + H_2O$

Stoichiometric Calculations

- Calculating the masses of products and the masses of reactants *requires*:
  - The **stoichiometric coefficients** from the balanced chemical equation.
  - Molar mass of the reactants.
  - Molar mass of the products.

Stoichiometry Example

- How much CO_2 enters the atmosphere annually from the combustion of 6.8×10^{12} kg of carbon?
- Balanced Eqn: $C(s) + O_2(g) \rightarrow CO_2(g)$
- 1mol C $\rightarrow$ 1mol CO2

$$6.8\times10^{12}\text{kg}\left(\frac{1000\text{ g}}{\text{kg}}\right)\left(\frac{1\text{ mole C}}{12\text{ g}}\right)\left(\frac{1\text{ mole CO}_2}{1\text{ mole C}}\right)\left(\frac{44.0\text{ g CO}_2}{1\text{ mole CO}_2}\right)\left(\frac{1\text{ kg}}{1000\text{ g}}\right)$$

From the stoichiometry; $1\text{mol C} \Rightarrow 1\text{mol CO}_2$

i.e. $12.0\text{g C} \Rightarrow 44.0\text{g CO}_2$

$$1.0\text{g C} \Rightarrow \frac{44.0}{12.0}\text{g CO}_2 = 3.67\text{g CO}_2$$

$$1.0\text{kg C} \Rightarrow 3.67\text{kg CO}_2$$

$$6.8\times10^{12}\text{kgC} \Rightarrow 6.8\times10^{12}\times3.67\text{kg CO}_2 = 2.50\times10^{13}\text{kg CO}_2$$

As a general method involving mass/mole calculations it is best to work in terms moles.

So convert mass to moles,
work in terms of moles (use stoichiometry/balanced equation),
convert back to mass (if need be).

Convert mass to moles;

$$6.8\times10^{12}\text{kgC} = \frac{6.8\times10^{12}\text{kg}}{12.0\times10^{-3}\text{kg/mol}}\text{C} = 5.67\times10^{14}\text{mol C}$$

From the stoichiometry; $1\text{molC} \Rightarrow 1\text{molCO}_2$

Therefore $5.67\times10^{14}\text{mol C} \Rightarrow 5.67\times10^{14}\text{mol CO}_2$

Convert moles to mass;

$$= 5.67\times10^{14}\text{mol CO}_2 \times \frac{44.0\text{gCO}_2}{1\text{molCO}_2} \times \frac{1\text{kg}}{10^3\text{g}} = 2.50\times10^{13}\text{kg}$$

Practice: Stoichiometry

How much carbon dioxide would be formed if 10.0 grams of C_5H_{12} were completely burned in oxygen?

$$C_5H_{12} + 8O_2 \rightarrow 5CO_2 + 6H_2O$$

Practice: Stoichiometry

Sodium carbonate reacts with hydrochloric acid to produce sodium chloride, water, and carbon dioxide. How much hydrochloric acid is required to produce 10.0 g of carbon dioxide?

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Mass Percent Composition from Molecular Formula

- Mass percent (%):

$$\frac{\text{mass of element in compound}}{\text{mass of compound}} \times 100\%$$

- Example: percent iron in iron(III) oxide (Fe_2O_3).

$$\% \text{ Fe in } Fe_2O_3 = \left(\frac{\text{mass Fe}}{\text{mass } Fe_2O_3}\right)\times 100 =$$

$$\left(\frac{(55.85 \text{ amu per Fe})(2 \text{ Fe atoms})}{159.7 \text{ amu per } Fe_2O_3 \text{ formula unit}}\right)\times 100 = 69.94\%$$

Empirical vs Molecular Formulas

- *Empirical Formula:*
  - Simplest whole-number molar ratio of elements in a compound.
- *Molecular Formula:*
  - Actual molar ratio of elements in a compound.
  - *Equal to a integral multiple of empirical formula:*
  - Need empirical formula and molecular formula.

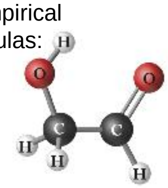
Empirical Formula: The simplest integral ratio of atoms in a compound.

e.g. A_mB_n: moles of A:moles of B = m:n

Molecular Formula		*Empirical Formula*
C_6H_6	C:H = 1:1	CH
Al_2O_3	Al:O = 2:3	Al_2O_3
Al_2Cl_6	Al:O = 1:3	$AlCl_3$

Empirical Formulas

- Many compounds have the same empirical formula, but different molecular formulas:
  - Glycoaldehyde (Fig. 3.19)
    - » Molecular = $C_2H_4O_2$
  - Glucose
    - » Molecular = $C_6H_{12}O_6$
  - Both compounds has the same Empirical formula
    - » Empirical formula: CH_2O



Molecular Formula = n (Empirical Formula)
Molar Mass = n (Empirical Mass)

Determination of Empirical Formula (EF):

Experimentally determine the masses or *mass percentages of each element* in the compound.

Implied here is if 100g of the compound is taken the mass of each element *in it* is equal to the percentage value in grams.

Ratio of mass(%) of elements
⇓ (Divide by atomic masses)
Ratio of moles of elements
⇓ (numerically equal to)
Ratio of Atoms (simplest integers!! ⇒ Empirical Formula)

if fractional,
I. Divide all values by smallest # in the ratio.
II. Bring numbers to the closest integers.

Repeat I and II if necessary.

In a given compound with C, H and O only;

% mass ratio; C : H : O = 40.92 : 4.58 : 54.50

mole ratio;
C:H:O = 40.92/12.00 : 4.58/1.00 : 54.50/16.00
C:H:O = 3.407 : 4.54 : 3.406
C:H:O = 1 : 1.33 : 1 !!!

Multiply by 3

C:H:O = 3 : 3.99 : 3 = 3 : 4 : 3 $\Rightarrow C_3H_4O_3$

Fractions and decimals:

$\frac{1}{2} = 0.50 \quad \frac{1}{3} = 0.33 \quad \frac{2}{3} = 0.67 \quad \frac{1}{4} = 0.25$

$\frac{3}{4} = 0.75 \quad \frac{1}{5} = 0.20 \quad \frac{2}{5} = 0.40 \quad \frac{3}{5} = 0.60$

$\frac{4}{5} = 0.80$ ....

Practice: Empirical Formulas

For thousands of years the mineral chalcocite has been a highly prized source of copper. Its chemical composition is 79.85% Cu and 20.15% S. What is its empirical formula?

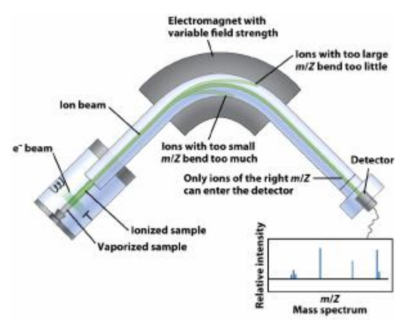
Practice: Empirical Formulas

Asbestos is a mineral containing magnesium, silicon, oxygen, and hydrogen. One form of asbestos, chrysotile (520.27 g/mol), has the composition 28.03% magnesium, 21.60% silicon, and the rest hydrogen. Determine the empirical formula of chrysotile.

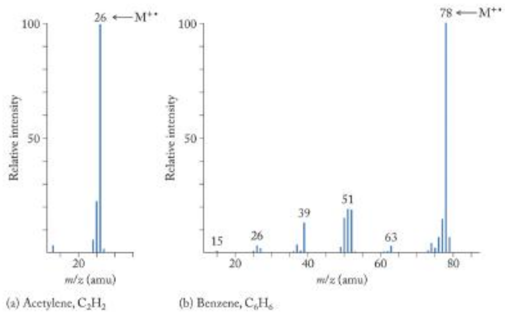
Mass Spectrometry and Molecular Mass

- To determine molecular formula you need, n:
  - Empirical mass & Molecular mass $\Rightarrow$ n.
- Mass spectrometers are instruments to determine the mass of substances.
  - Convert molecules into ions.
  - Separate ions based on mass/charge ratio.

Mass Spectrometer



Mass Spectra



$$n = \frac{\text{Molecular Formula}}{\text{Empirical Formula}}$$

$$n = \frac{\text{Molar Mass (g)}}{\text{Empirical Mass (g)}}$$

$$n = \frac{\text{Molecular Mass(amu)}}{\text{Mass of Empirical unit(amu)}}$$

Determining the Molecular Formula

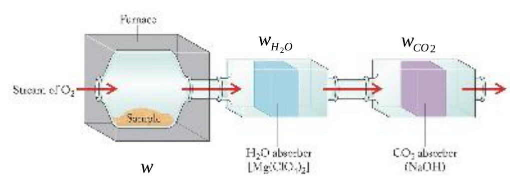
- Molecular formula determined from:
  - Mass % composition ⇒ (empirical formula).
  - Mass spectral data (molecular mass).
- Example:

Compound	Empirical Formula	Molecular Mass		Molecular Formula
Acetylene	CH (13 amu)	26 amu	(EF × 2)	C_2H_2
Benzene	CH (13 amu)	78 amu	(EF × 6)	C_6H_6

Combustion Analysis for % Composition

The percent of carbon and hydrogen in C_aH_b can be determined from the mass of H_2O and CO_2 produced by combustion:

C_aH_b + excess O_2 → $a CO_2(g) + (b/2) H_2O$



Wt. H in sample:

$$w_H = w_{H2O} \times \frac{1 mol H_2O}{18.015 g H_2O} \times \frac{2 mol H}{1 mol H_2O} \times \frac{1.0079 g H}{1 mol H}$$

Wt. C in sample:

$$w_C = w_{CO2} \times \frac{1 mol CO_2}{44.009 g CO_2} \times \frac{1 mol C}{1 mol CO_2} \times \frac{12.011 g C}{1 mol C}$$

Wt. O in sample:

$$w_O = w - (w_C + w_H)$$

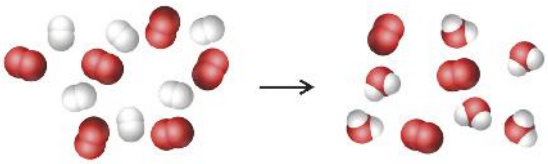
Practice: Combustion Analysis

Combustion analysis of an unknown compound indicated that it is 92.23% C and 7.82% H. The mass spectrum indicated the molar mass is 78 g/mol. What is the molecular formula of this unknown compound?

Limiting Reactants/Reagent

Hydrogen and Oxygen react to form water:

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$



H_2 (g) = white; O_2(g) = red. Which runs out first?

Limiting Reactants/Reagent

- Limiting Reactant:
  - Substance that is *completely consumed* in the chemical reaction.
  - *Determines the amount of product* that can be formed during the reaction.
  - Identified by:
    1. number of moles of reactants mixed
    2. *stoichiometry of balanced chemical equation*

Identifying Limiting Reactants/Reagent

1. Write the balanced chemical equation.
2. Calculate the # moles of a reactants used (given) or the reaction.
3. Calculate the # moles of a product based on each reactant (in the step above).
4. The reactant that makes the least # moles of product is the limiting reagent/reactant.

Practice: Limiting Reactant

If 10.0 g of methane (CH_4) is burned in 20.0 g of oxygen (O_2) to produce carbon dioxide (CO_2) and water (H_2O):

a) What is the limiting reactant?
b) How many grams of water will be produced?

Percent Yield

- Theoretical Yield:
  - The calculated amount of product formed based on the amount of limiting reactant.
- Actual Yield:
  - The actual measured amount of product formed.

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\%$$

Practice: Percent Yield

Aluminum burns in bromine liquid, producing aluminum bromide. In one experiment, 6.0 g of aluminum reacted with an excess of bromine to yield 50.3 g aluminum bromide. Calculate the theoretical and percent yields.

Sample Exercise 3.1

It's not unusual for the polluted air above a large metropolitan area to contain as much as 5×10^{-10} moles of SO_2 per liter of air. What is this concentration of SO_2 in molecules per liter?

$$\frac{5 \times 10^{-10}\ \text{mol } SO_2}{1\ \text{L air}} \times \frac{6.022 \times 10^{23}\ \text{molecules } SO_2}{1\ \text{mol } SO_2} = \frac{3 \times 10^{14}\ \text{molecules } SO_2}{1\ \text{L air}}$$

Sample Exercise 3.2

Some antacid tablets contain 425 mg of calcium (as Ca^{2+} ions). How many moles of calcium are in each tablet? (The average atomic mass of an atom of calcium is 40.078 amu, which means the molar mass of calcium is 40.08 g/mol when rounded to four significant figures.[1])

$$425\ \text{mg } Ca^{2+} \times \frac{1\ \text{g}}{10^3\ \text{mg}} \times \frac{1\ \text{mol } Ca^{2+}}{40.08\ \text{g } Ca^{2+}} = 0.0106\ \text{mol } Ca^{2+}$$

Sample Exercise 3.5

Calculate the number of moles and the number of formula units of calcium carbonate contained in 1.28 g of $CaCO_3$.

Sample Exercise 3.5 (cont.)

First determine the formula mass of

40.08 g/mol + 12.01 g/mol + 3(16.00 g/mol) = 100.09 g/mol $CaCO_3$
Converting from grams $CaCO_3$ to moles $CaCO_3$ gives

$$1.28\ \text{g } CaCO_3 \times \frac{1\ \text{mol } CaCO_3}{100.09\ \text{g } CaCO_3} = 0.01279\ \text{mol } CaCO_3$$

Carrying on the calculation with the intermediate value and multiplying by Avogadro's number gives

$$0.01279\ \text{mol } CaCO_3 \times \frac{6.022 \times 10^{23}\ \text{formula units } CaCO_3}{1\ \text{mol } CaCO_3} = 7.702 \times 10^{21}\ \text{formula units } CaCO_3$$

The final answer must have three significant figures, so the number of formula units of $CaCO_3$ is 7.70×10^{21}.

Sample Exercise 3.9

What is the percent composition of the mineral forsterite, Mg_2SiO_4?

Sample Exercise 3.9 (cont.)

To calculate the percent dividing the mass of each element in 1 mole of forsterite by the molar mass of forsterite.

The molar mass of Mg_2SiO_4 = 140.71 g/mol
The percent composition of this compound is therefore

$$\%Mg = \frac{48.62\ \text{g Mg}}{140.71\ \text{g}} \times 100\% = 34.55\%\ \text{Mg}$$
$$\%Si = \frac{28.09\ \text{g Si}}{140.71\ \text{g}} \times 100\% = 19.96\%\ \text{Si}$$
$$\%O = \frac{64.00\ \text{g O}}{140.71\ \text{g}} \times 100\% = 45.48\%\ \text{O}$$