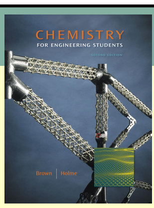

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Chapter 3
Molecules, Moles, and Chemical Equations

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Warning!!

- These slides contains visual aids for learning BUT they are NOT the actual lecture notes!
- Failure to attend to lectures most probably result in failing the lecture!
- So I strongly recommend that you attend to the classes. Take a pen, a notebook and WRITE!

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Chapter Objectives

- List at least three characteristics of explosive chemical reactions.
- Explain balancing a chemical reaction as an application of the law of conservation of mass.
- List at least three quantities that must be conserved in chemical reactions.
- Write balanced chemical equations for simple reactions, given either an unbalanced equation or a verbal description.

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Chapter Objectives

- Explain the concept of a mole in your own words.
- Interpret chemical equations in terms of both moles and molecules.
- Interconvert between mass, number of molecules, and number of moles.
- Determine a chemical formula from elemental analysis (i.e., from % compositions).

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Chapter Objectives

- Define the concentration of a solution and calculate the molarity of solutions from appropriate data.
- Calculate the molarity of solutions prepared by dilution or calculate the quantities needed to carry out a dilution to prepare a solution of a specified concentration.
- Distinguish between electrolytes and nonelectrolytes and explain how their solutions differ.

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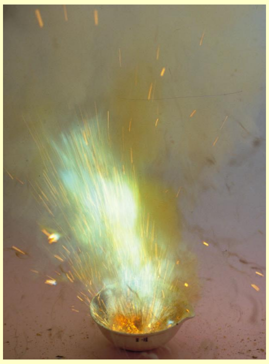
Chapter Objectives

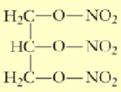
- Describe the species expected to be present (ions, molecules, etc.) in various simple solutions.
- Recognize common strong acids and bases.
- Write molecular and ionic equations for acid-base neutralization reactions.

Explosions

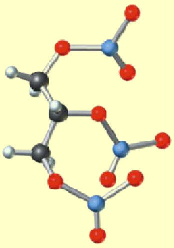
1. Explosions release a large amount of energy when a fairly complex molecule decomposes into smaller, simpler compounds.
2. Explosions occur very quickly.
3. Modern explosives are generally solids.



Explosions

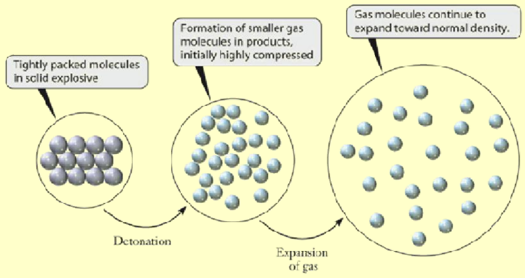


Nitroglycerin



- Dynamite is an explosive made from liquid nitroglycerin and an inert binder to form a solid material.
  - Solids are easier to handle than liquids

Explosions



- The destructive force of explosions is due in part to expansion of gases, which produces a shockwave.

Chemical Formulas and Equations

- Chemical formulas provide a concise way to represent chemical compounds.
  - Nitroglycerin, shown earlier, becomes $C_3H_5N_3O_9$
- A chemical equation builds upon chemical formulas to concisely represent a chemical reaction.

Writing Chemical Equations

- Chemical equations represent the transformation of one or more chemical species into new substances.
  - Reactants are the original materials and are written on the left hand side of the equation.
  - Products are the newly formed compounds and are written on the right hand side of the equation.

Reactants → Products

Writing Chemical Equations

- Chemical formulas represent reactants and products.
- Phase labels follow each formula.
  - solid = (s)
  - liquid = (ℓ)
  - gas = (g)
  - aqueous (substance dissolved in water) = (aq)
- Some reactions require an additional symbol placed over the reaction arrow to specify reaction conditions.
  - Thermal reactions: heat (Δ)
  - Photochemical reactions: light ($h\nu$)

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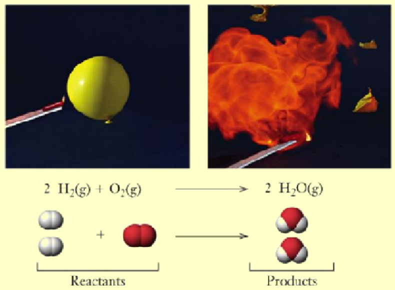
Writing Chemical Equations



- Different representations for the reaction between hydrogen and oxygen to produce water.

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Balancing Chemical Equations

- The law of conservation of matter: matter is neither created nor destroyed.
  - Chemical reactions must obey the law of conservation of matter.
    - The same number of atoms for each element must occur on both sides of the chemical equation.
    - A chemical reaction simply rearranges the atoms into new compounds.

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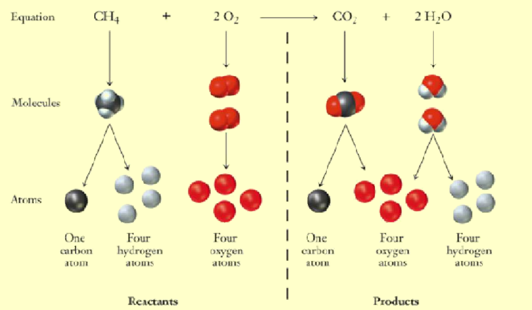
Balancing Chemical Equations



- Balanced chemical equation for the combustion of methane.

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Balancing Chemical Equations

- Chemical equations may be balanced via inspection, which really means by trial and error.
  - Numbers used to balance chemical equations are called stoichiometric coefficients.
    - The stoichiometric coefficient multiplies the number of atoms of each element in the formula unit of the compound that it precedes.
  - Stoichiometry is the various quantitative relationships between reactants and products.

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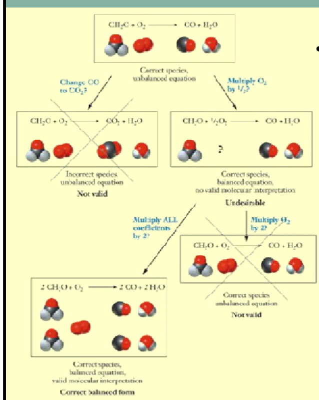
Balancing Chemical Equations



- Pay attention to the following when balancing chemical equations:
  - Do not change species
  - Do not use fractions (cannot have half a molecule)
  - Make sure you have the same number of atoms of each element on both sides

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Example Problem 3.1

- Write a balanced chemical equation describing the reaction between propane, C_3H_8, and oxygen, O_2, to form carbon dioxide and water.

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Aqueous Solutions and Net Ionic Equations

- Reactions that occur in water are said to take place in aqueous solution.
  - Solution: homogeneous mixture of two or more substances.
    - Solvent: solution component present in greatest amount.
    - Solute: solution component present in lesser amount.
    - The preparation of a solution is a common way to enable two solids to make contact with one another.

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Solutions, Solvents, and Solutes

- For solutions, the concentration is a key piece of information.
  - Concentration: relative amounts of solute and solvent.
  - Concentrated: many solute particles are present.
  - Dilute: few solute particles are present.

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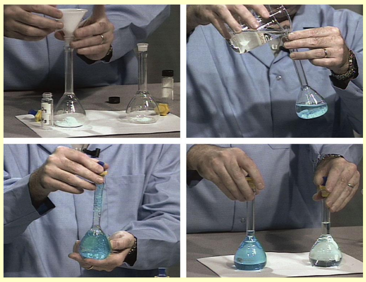
Solutions, Solvents, and Solutes

Solution preparation:

- Solid $CuSO_4$, the solute, is transferred to a flask.
- Water, the solvent, is added.
- The flask is shaken to speed the dissolution process.
- Two solutions of $CuSO_4$.
  - Solution on the left is more concentrated, as seen from its darker color.



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Solutions, Solvents, and Solutes

- Compounds can be characterized by their solubility.
  - Soluble compounds dissolve readily in water.
  - Insoluble compounds do not readily dissolve in water.
- Solubility can be predicted using solubility guidelines.

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Solutions, Solvents, and Solutes

- Solubility guidelines for soluble salts

Table 3.1

Solubility guidelines for ionic compounds in water at room temperature

Usually Soluble	Exceptions
Group 1 cations (Li^+, Na^+, K^+, Rb^+, Cs^+), ammonium (NH_4^+)	No common exceptions
Nitrates (NO_3^-), nitrites (NO_2^-)	Moderately soluble: $AgNO_2$
Chlorides, bromides, iodides (Cl^-, Br^-, I^-)	Insoluble: $AgCl$, Hg_2Cl_2, $PbCl_2$, $AgBr$, Hg_2Br_2, $PbBr_2$, AgI, Hg_2I_2, and PbI_2
Fluorides (F^-)	Insoluble: MgF_2, CaF_2, SrF_2, BaF_2, PbF_2
Sulfates (SO_4^{2-})	Insoluble: $BaSO_4$, $PbSO_4$, $HgSO_4$ Moderately soluble: $CaSO_4$, $SrSO_4$, Ag_2SO_4
Chlorates (ClO_3^-), perchlorates (ClO_4^-)	No common exceptions
Acetates (CH_3COO^-)	Moderately soluble: $AgCH_3COO$

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Solutions, Solvents, and Solutes

- Solubility guidelines for insoluble salts

Table 3.1

Solubility guidelines for ionic compounds in water at room temperature

Usually Insoluble	Exceptions
Phosphates (PO_4^{3-})	Soluble: $(NH_4)_3PO_4$, Na_3PO_4, K_3PO_4
Carbonates (CO_3^{2-})	Soluble: $(NH_4)_2CO_3$, Na_2CO_3, K_2CO_3
Hydroxides (OH^-)	Soluble: LiOH, NaOH, KOH, $Ba(OH)_2$ Moderately soluble: $Ca(OH)_2$, $Sr(OH)_2$
Sulfides (S^{2-})	Soluble: $(NH_4)_2S$, Na_2S, K_2S, MgS, CaS

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Example Problem 3.2

- Which of the following compounds would you predict are soluble in water at room temperature?

a) $KClO_3$

b) $CaCO_3$

c) $BaSO_4$

d) $KMnO_4$

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Solutions, Solvents, and Solutes

- Electrolytes are soluble compounds that conduct current when dissolved in water.
  - Weak electrolytes dissociate partially into ions in solution.
  - Strong electrolytes dissociate completely into ions in solution.
- Nonelectrolytes do not dissociate into ions in solution.

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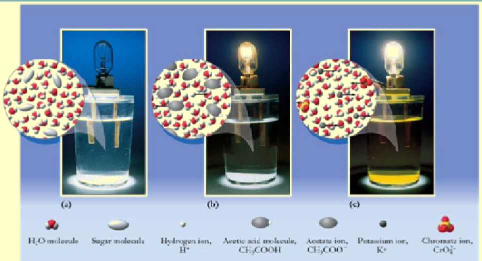
Solutions, Solvents, and Solutes



a) Sugar, a nonelectrolyte, does not conduct current when dissolved in water.
b) Acetic acid, a weak electrolyte, weakly conducts current when dissolved in water.
c) Potassium chromate, a strong electrolyte, strongly conducts current when dissolved in water.

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Chemical Equations for Aqueous Reactions

- When a covalently bonded material dissolves in water and the molecules remain intact, they do not conduct current. These compounds are nonelectrolytes.

$$C_6H_{12}O_6\ (s) \longrightarrow C_6H_{12}O_6\ (aq)$$

  - The water molecules are not shown explicitly, although their presence is indicated by the "(aq)" on the product side.

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Chemical Equations for Aqueous Reactions

- When an ionic solid dissolves in water, it breaks into its constituent ions. This is called a dissociation reaction. These compounds conduct electric current and are electrolytes.

$$NaCl\ (s) \longrightarrow Na^+\ (aq) + Cl^-\ (aq)$$

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Chemical Equations for Aqueous Reactions

- Aqueous chemical reactions can be written as a molecular equation. The complete formula for each compound is shown.
  - Note, all of the species may not be molecules.

$$HNO_3(aq) + NH_3(g) \longrightarrow NH_4NO_3(aq)$$

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Chemical Equations for Aqueous Reactions

- Dissociation of reactants and products is emphasized by writing a total ionic equation.

$$H^+(aq) + NO_3^-(aq) + NH_3(g) \longrightarrow NH_4^+(aq) + NO_3^-(aq)$$

- Note: HNO_3 is a strong acid and thus dissociates completely, while NH_3 does not dissociate

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Chemical Equations for Aqueous Reactions

- Spectator ions are ions uninvolved in the chemical reaction. When spectator ions are removed, the result is the net ionic equation.
  - Total ionic equation

$$H^+(aq) + NO_3^-(aq) + NH_3(g) \longrightarrow NH_4^+(aq) + NO_3^-(aq)$$

  - Net ionic equation

$$H^+(aq) + NH_3(g) \longrightarrow NH_4^+(aq)$$

$$\text{Spectator ion} = NO_3^-$$

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Acid-Base Reactions

- Acids are substances that dissolve in water to produce H^+ (or H_3O^+) ions.
  - Examples: HCl, HNO_3, H_3PO_4, HCN
- Bases are substances that dissolve in water to produce OH^- ions.
  - Examples: NaOH, $Ca(OH)_2$, NH_3

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Acid-Base Reactions

- Strong acids and bases completely dissociate in water.

$$HCl(g) + H_2O(l) \longrightarrow H_3O^+(aq) + Cl^-(aq)$$

$$NaOH(s) \longrightarrow Na^+(aq) + OH^-(aq)$$

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Acid-Base Reactions

- *All* common strong acids and bases.

Table 3.2

Strong and weak acids and bases

Strong Acids		Strong Bases	
HCl	Hydrochloric acid	LiOH	Lithium hydroxide
HNO_3	Nitric acid	NaOH	Sodium hydroxide
H_2SO_4	Sulfuric acid	KOH	Potassium hydroxide
$HClO_4$	Perchloric acid	$Ca(OH)_2$	Calcium hydroxide
HBr	Hydrobromic acid	$Ba(OH)_2$	Barium hydroxide
HI	Hydriodic acid	$Sr(OH)_2$	Strontium hydroxide

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Acid-Base Reactions

- Weak acids and bases partially dissociate in water.
  - Notice the two-way arrows, which emphasize that the reaction does not proceed completely from left to right.

$$CH_3COOH(aq) + H_2O(l) \rightleftarrows H_3O^+(aq) + CH_3COO^-(aq)$$

$$NH_3(aq) + H_2O(l) \rightleftarrows NH_4^+(aq) + OH^-(aq)$$

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Acid-Base Reactions

- *Some* common weak acids and bases.

Table 3.2

Strong and weak acids and bases

Weak Acids		Weak Bases	
H_3PO_4	Phosphoric acid	NH_3	Ammonia
HF	Hydrofluoric acid	CH_3NH_2	Methylamine
CH_3COOH	Acetic acid		
HCN	Hydrocyanic acid		

Note: *All* common strong acids and bases are shown, but only representative examples of weak acids and bases are listed.

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Acid-Base Reactions

- Mixing an acid and a base leads to a reaction known as neutralization, in which the resulting solution is neither acidic nor basic.
  - Net ionic equation for neutralization of strong acid and strong base.

$$H_3O^+(aq) + OH^-(aq) \longrightarrow 2H_2O(l)$$

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Example Problem 3.3

- When aqueous solutions of acetic acid and potassium hydroxide are combined, a neutralization reaction will occur. Write the following equations:

a) molecular

b) total ionic

c) net ionic

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Precipitation Reactions

- A precipitation reaction is an aqueous reaction that produces a solid, called a precipitate.
  - Net ionic reaction for the precipitation of lead(II) iodide.

$$Pb^{2+}(aq) + 2I^-(aq) \longrightarrow PbI_2(s)$$

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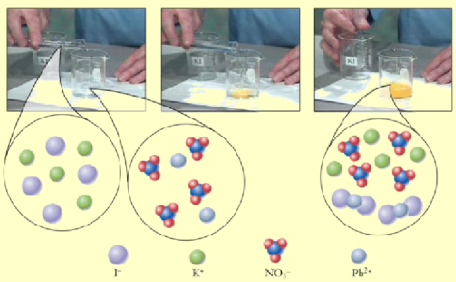
Precipitation Reactions



- Precipitation reaction between aqueous solutions of KI and $Pb(NO_3)_2$, which are both colorless.
- The bright yellow solid, PbI_2, is produced.
- PbI_2 is insoluble as predicted by the solubility guidelines.

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Example Problem 3.4

- When aqueous sodium carbonate and barium chloride are combined, the solution becomes cloudy white with solid barium carbonate. Write the following equations:

  a) molecular

  b) total ionic

  c) net ionic

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Interpreting Equations and the Mole

- Balanced chemical equations are interpreted on the microscopic and macroscopic level.
  - Microscopic interpretation visualizes reactions between molecules.
  - Macroscopic interpretation visualizes reactions between bulk materials.

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Interpreting Chemical Equations

- Balanced chemical reactions provide stoichiometric ratios between reactants and products. Ratios relate relative numbers of particles.

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

  - 2 molecules H_2 : 1 molecule O_2 : 2 molecules H_2O
  - 100 molecules H_2 : 50 molecule O_2 : 100 molecules H_2O

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Avogadro's Number and the Mole

- A mole is a means of counting the large number of particles in samples.
  - One mole is the number of atoms in exactly 12 grams of ^{12}C (carbon-12).
  - 1 mole contains Avogadro's number (6.022×10^{23} particles/mole) of particles.
  - The mass of 6.022×10^{23} atoms of any element is the molar mass of that element.

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Avogadro's Number and the Mole

- One mole samples of various elements. All have the same number of particles.

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Avogadro's Number and the Mole

- Balanced chemical reactions also provide mole ratios between reactants and products.

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

  - 2 moles H_2 : 1 mole O_2 : 2 moles H_2O

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Determining Molar Mass

- The molar mass of a compound is the sum of the molar masses of all the atoms in a compound.

$$\left(2 \text{ mol H} \times \frac{1.0 \text{ g H}}{1 \text{ mol H}}\right) + \left(1 \text{ mol O} \times \frac{16.0 \text{ g}}{1 \text{ mol O}}\right)$$

$$= 18.0 \text{ g/mol } H_2O$$

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Example Problem 3.5

- Determine the molar mass of each of the following compounds:

a) PbN_6

b) $C_3H_5N_3O_9$

c) $Hg(ONC)_2$

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Calculations Using Moles and Molar Mass

- *Molar mass allows conversion from mass to number of moles, much like a unit conversion.*
  - 1 mol $C_7H_5N_3O_6$ = 227.133 g $C_7H_5N_3O_6$

$$300.0 \text{ g } C_7H_5N_3O_6 \times \frac{1 \text{ mol } C_7H_5N_3O_6}{227.133 \text{ g } C_7H_5N_3O_6}$$

$$= 1.320 \text{ mol } C_7H_5N_3O_6$$

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Calculations Using Moles and Molar Mass

- *Avogadro's number functions much like a unit conversion between moles to number of particles.*
  - 1 mol $C_7H_5N_3O_6$ = 6.022×10^{23} $C_7H_5N_3O_6$ molecules
  - How many molecules are in 1.320 moles of nitroglycerin?

$$1.320 \text{ mol } C_7H_5N_3O_6 \times \frac{6.022 \times 10^{23} \text{ molecules } C_7H_5N_3O_6}{1 \text{ mol } C_7H_5N_3O_6}$$

$$= 7.949 \times 10^{23} \text{ molecules } C_7H_5N_3O_6$$

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Example Problem 3.6

- A sample of the explosive TNT ($C_7H_5N_3O_6$) has a mass of 650.5 g.
  - How many moles of TNT are in this sample?
  - How many molecules are in this sample?

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Example Problem 3.7

- How many pounds of halite ($C_2H_6N_4O_5$) correspond to 315 moles? (1 pound = 454 g)

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Elemental Analysis: Determining Empirical and Molecular Formulas

- Empirical formulas can be determined from an elemental analysis.
  - An elemental analysis measures the mass percentage of each element in a compound.
  - The formula describes the composition in terms of the number of atoms of each element.
  - The molar masses of the elements provide the connection between the elemental analysis and the formula.

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Elemental Analysis: Determining Empirical and Molecular Formulas

- Assume a 100 gram sample size
- Percentage element × sample size = mass element in compound. (e.g., 16% carbon = 16 g carbon)
- Convert mass of each element to moles using the molar mass.
- Divide by smallest number of moles to get mole to mole ratio for empirical formula.
- When division by smallest number of moles results in small rational fractions, multiply all ratios by an appropriate integer to give whole numbers.
  - 2.5 × 2 = 5, 1.33 × 3 = 4, etc.

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Example Problem 3.8

- The explosive known as RDX contains 16.22% carbon, 2.72% hydrogen, 37.84% nitrogen, and 43.22% oxygen by mass. Determine its empirical formula.

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Elemental Analysis: Determining Empirical and Molecular Formulas

- A molecular formula is a whole number multiple of the empirical formula.
  - Molar mass for the molecular formula is a whole number multiple of the molar mass for the empirical formula.
  - If the empirical formula of a compound is CH_2 and its molar mass is 42 g/mol, what is its molecular formula?

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Example Problem 3.9

- An alloy contains 70.8 mol % palladium and 29.2 mol % nickel. Express the composition of this alloy as weight percentage (wt %).

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Molarity

- Molarity, or molar concentration, *M*, is the number of moles of solute per liter of solution.
  - Provides relationship among molarity, moles solute, and liters solution.

$$\text{Molarity } (M) = \frac{\text{moles of solute}}{\text{liter of solution}}$$

  - If we know any two of these quantities, we can determine the third.

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Example Problem 3.10

- A solution is prepared by dissolving 45.0 g of NaClO in enough water to produce exactly 750 mL of solution. What is the molarity of this solution?

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Dilution

- Dilution is the process in which solvent is added to a solution to decrease the concentration of the solution.
    - The number of moles of solute is the same before and after dilution.
    - Since the number of moles of solute equals the product of molarity and volume ($M \times V$), we can write the following equation, where the subscripts denote initial and final values.

$$M_{\mathrm{i}} \times V_{\mathrm{i}} = M_{\mathrm{f}} \times V_{\mathrm{f}}$$

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Example Problem 3.11

- A chemist requires 1.5 M hydrochloric acid, HCl, for a series of reactions. The only solution available is 6.0 M HCl. What volume of 6.0 M HCl must be diluted to obtain 5.0 L of 1.5 M HCl?

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Explosive and Green Chemistry

- Green chemistry: the philosophy that chemical processes and products should be designed with the goal of reducing environmental impacts
    - Firing of guns involves detonating a primer, which then induces a larger explosion.
        - Traditional primers are lead-based, e.g., $Pb(N_3)_2$
        - Research is underway to find less toxic primers

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