# CHAPTER 3
# FORMULAS, EQUATIONS, AND MOLES

## Chapter Learning Goals

**Section 3.1** For simple chemical reactions, write and balance chemical equations.

**Section 3.2** Differentiate between microscopic and macroscopic interpretations of chemical formulas.

**Section 3.3** Determine the formula of a compound from its ball-and-stick model.

Calculate molar mass.

**Section 3.4** Interconvert grams, moles, and numbers of formula units.

Determine the number of moles and grams of one reactant needed to react with a given number of moles and grams of another reactant and the number of moles and grams of product(s) that result from the reaction.

**Section 3.5** Calculate percent yield.

Calculate the number of grams of products produced from a given number of grams of reactants when the theoretical yield is less than 100%.

**Section 3.6** Identify the limiting and excess reagents in a reaction mixture.

Determine the number of grams of excess reagent remaining at the end of a reaction and the number of grams of product(s) produced.

**Section 3.7** Describe how to prepare a solution of known molarity by dissolving a solid in a solvent.

Calculate the number of moles of solute in a given volume of solution and vice versa.

**Section 3.8** Describe how to prepare a solution of known molarity by diluting a more concentrated solution.

Determine the final concentration of solution after dilution.

**Section 3.9** Interconvert solution molarity, solution volume, solute moles, and solute grams.

**Section 3.10** Determine the volume of one reactant needed to react with a given volume of a second reactant.

Determine the molarity of an acid or base solution by titration.

**Section 3.11** Determine the percent composition and empirical formula of a compound.

**Section 3.12** Use combustion analysis data to obtain the empirical formula of a compound containing carbon, hydrogen, and one other element.

From empirical formula and molar mass, determine the molecular formula of a compound.

**Section 3.13** Describe how atomic and molecular masses can be determined by mass spectrometry.

## Lecture Outline

**3.1. Balancing Chemical Equations**

A. Balanced equations
  1. Numbers and species of atoms on both sides of the arrow are equal
  2. Chemical equations balanced to obey law of mass conservation

B. Formula unit – one unit (an atom, ion, or molecule) corresponding to a given formula

C. Balancing process
  1. Write unbalanced equation using correct chemical formulas for all reactants and products
  2. Use coefficients (numbers placed before each formula) to indicate number of formula units required to balance the equation
     a. Coefficients can be changed
     b. Formulas of all reactants and products remain the same
  3. Reduce coefficients to smallest whole numbers
  4. Check your answer
  5. When balancing chemical equations involving organic compounds (compounds of carbon), balance the atoms in the order C then H then O.

**3.2. Chemical Symbols on Different Levels**

A. Chemical symbols – represent both a microscopic and a macroscopic level

B. Microscopic level – chemical symbols represent behavior of individual atoms and molecules

C. Macroscopic level – formulas and equations represent large-scale behavior of atoms and molecules giving rise to observable properties
  1. Deal with macroscopic behavior in the laboratory
  2. Use microscopic models to explain macroscopic behavior

**3.3. Avogadro's Number and the Mole**

A. Dealing with macroscopic behavior requires that the number ratio of reactants or products from a balanced equation be converted to a mass ratio (In the laboratory we do not count numbers of atoms, we weigh grams of reactants and products.)
  1. Number ratio determined from coefficients in the balanced equation
  2. Mass ratio determined using molecular masses (molecular weights)
     a. Molecular mass – sum of atomic masses of all atoms in a molecule
     b. Formula mass – sum of atomic masses of all atoms in one formula unit of any substance

B. Mass ratio of molecules (or formula units) = molecular (or formula unit) mass ratio

C. One mole of any substance is the amount whose mass is equal to the molecular or formula mass in grams.
  1. Mole (mol) = $6.022 \times 10^{23}$ particles
     a. Avogadro's number (abbreviated $N_A$)
     b. 1 mol $HNO_3$ = $6.022 \times 10^{23}$ molecules of $HNO_3$
     c. 1 mol electrons = $6.022 \times 10^{23}$ electrons
  2. Importance of mole – provides a relationship between numbers of molecules and masses of molecules

D. Molar mass of a substance – one mole of any substance has a mass equal to its molecular or formula mass in grams
  1. Mass of one mole of a substance
  2. Mass of $6.022 \times 10^{23}$ molecules, ions, atoms, or compounds
  3. Molecular mass of substance in grams
  4. Serves as a conversion factor between numbers of formula units and mass
  5. Formula of the particles is always specified, i.e., 18.0 g $H_2O$/mol $H_2O$

E. Coefficients in a balanced chemical equation indicate the number of moles of each substance needed for the reaction. Coefficients do not represent grams or mass of formula units.

**3.4. Stoichiometry: Chemical Arithmetic**

A. Stoichiometry – refers to the conversion between moles and grams of reactants and products in a chemical equation

B. Converting grams, moles and formula units – use the molar mass of the substance as a conversion factor, remembering significant figures.
C. Calculating the grams of reactants needed and products produced, knowing the grams and moles of another reactant
   1. Begin with the known grams of reactant, convert to moles
   2. Using the balanced chemical equation, convert moles of one substance to moles of another
   3. Knowing moles, convert to grams

**3.5. Yields of Chemical Reactions**

A. Actual yield – an experimental quantity that cannot be calculated.
   1. Amount of product actually formed
   2. Less than the amount predicted by theory
B. Theoretical yield – amount of product calculated to form if all of the reactants are converted to products
C. $\text{Percent yield} = \dfrac{\text{Actual yield}}{\text{Theorectical yield}} \times 100\%$

**3.6. Reactions with Limiting Amounts of Reactants**

A. Many reactions carried out using an excess of one reactant
B. Excess reactant – reactant present with more moles than needed according to the stoichiometry. Not necessarily the reactant present in greatest mass.
   1. Only amount required by stoichiometry reacts
   2. Excess reactant acts as a spectator and plays no role in the reaction
C. Limiting reactant
   1. Reactant present in an insufficient molar amount as required by stoichiometry for complete reaction.
   2. Determines the extent to which a chemical reaction takes place – how much can be produced.
   3. Reaction stops when limiting reactant depleted
D. Methods to determine limiting reactant:
   1. Compare stoichiometric ratio to actual ratio of moles for reactants
   2. Determine theoretical yield based on each reactant
   3. Determine amount of one reactant needed to react with given quantity of other reactants
E. Determination of whether a limiting amount of one reactant is present and calculation of the amount of excess reactant remaining:
   1. Find moles of each reactant present
   2. Look at the coefficients in the balanced equation to find the required mole ratio of the two reactants – compare to number of moles calculated in the first step
   3. Subtract number of moles of excess reactant consumed from the number of moles of excess reactant present.
      a. Convert to grams
      b. This is grams of nonlimiting reactant in excess
   4. Determination of the amount of product formed:
      a. Base on moles of limiting reactant
      b. Moles limiting reactant $\rightarrow$ moles product $\rightarrow$ grams product

**3.7. Concentrations of Reactants in Solution: Molarity**

A. Most chemical reactions carried out in solution – reactants must have considerable mobility for reaction to occur
B. Solute – substance dissolved in a solvent to make a solution
C. Concentration – relative amount of solute to solvent or in solution
D. Molarity (M) – number of moles of a solute dissolved in each liter of solution, not solvent
   1. Dissolve solute in enough solution to give a final solution volume of 1.00 L
   2. Used as conversion factor

**3.8. Diluting Concentrated Solutions**

A. Concentrated solution + Solvent $\rightarrow$ Diluted solution

B. Dilution
1. Number of moles of solute remains the same
2. Only volume is changed by adding more solvent
3. A convenient relationship:

$$\text{Moles of solute} = M_i\left(\frac{\text{mol}}{\text{L}}\right)\times V_i\,(\text{L}) = M_f\left(\frac{\text{mol}}{\text{L}}\right)\times V_f\,(\text{L})$$

4. Note: This equation should be used only for problems that deal with dilution of a solution! Does not work for stoichiometry problems.

**3.9. Solution Stoichiometry**

A. Knowing the molarity of solutions is important when performing stoichiometry calculations on substances in solution

B. Use molarity to calculate either the number of moles (if volume is known) or volume (if the number of moles is known)

**3.10. Titration**

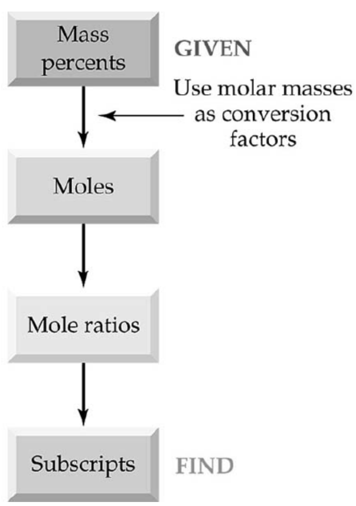
A. Procedure for determining the concentration of a solution

B. Carefully measured volume of one solution reacts with a second solution of known concentration and volume

**3.11. Percent Composition and Empirical Formulas**

A. Composition of a compound – identity and amount of elements present in a compound

B. Percent composition
1. Mass percent of each element present in a compound
2. Calculation of chemical formula from percent composition:
   a. Find relative numbers of moles of each element in the compound.
      i. Assume 100 g of compound
      ii. Use molar masses of elements as conversion factors
   b. Find ratio of the numbers of moles by dividing larger number of moles by smaller number of moles. Note: experimental or calculation errors may result in mole ratios that are not exactly whole numbers.
   c. Multiply subscripts by small integers in a trial-and-error procedure until whole numbers found




C. Empirical formula – gives only ratios of atoms in a compound

D. Molecular formula – gives actual numbers of atoms in a molecule
1. May be the same as the empirical formula
2. May be a multiple of the empirical formula:

$$\text{Multiple} = \frac{\text{Molecular mass}}{\text{Empirical formula mass}}$$

E. Derive percent composition from chemical formula

**3.12. Determining Empirical Formulas: Elemental Analysis**

A. Combustion analysis – compound of unknown composition burned with oxygen to produce volatile combustion products $CO_2$ and $H_2O$
  1. $CO_2$ and $H_2O$ separated by a gas chromatograph and their masses determined
  2. Used to determine empirical formula of a compound

B. Determination of empirical formula of a compound from combustion reaction:
  1. Perform gram-to-mole conversions to find molar amounts of C and H in $CO_2$ and $H_2O$
  2. Perform mole-to-gram conversions to find number of grams of C and H in original sample
  3. Subtract masses of C and H from the mass of starting sample to determine number of grams of third element
  4. Determine number of moles of third element
  5. Find mole ratios by dividing larger number of moles by smaller number of moles

C. Determination of molecular formula of a substance:
  1. Molecular mass determined from a separate experiment (e.g., using mass spectrometry)
  2. Subscripts in empirical formula multiplied by ratio of molecular mass to empirical formula mass

**3.13. Determining Molecular Masses: Mass Spectrometry**

A. Most common method for molecular mass determination

B. Method
  1. Vaporized sample ionized by bombardment with high-energy electrons
  2. Some molecular ions fragment into smaller ions
  3. Rapidly-moving ions pass through a curved magnetic field
     a. Pathway followed by ions mass-dependent
     b. Lighter ions deflected more strongly than heavier ions
  4. Ions separated by mass enter a detector assembly
     a. Signal intensities proportional to the relative number of each ion
     b. Mass of each ion assigned by comparison to a standard
  5. Very precise – molecular masses determined to as many as seven significant figures