3.1 Chemical Equations

- Lavoisier observed that mass is conserved in a chemical reaction.
  - This observation is known as the **law of conservation of mass**.
- The quantitative nature of chemical formulas and reactions is called **stoichiometry**.
- **Chemical equations** give a description of a chemical reaction.
- **There are two parts to any equation:**
  - **Reactants** (written to the left of the arrow) and
  - **Products** (written to the right of the arrow):

$$2\ H_2 + O_2 \dashrightarrow 2\ H_2O$$

- There are two sets of numbers in a chemical equation:
  - Numbers in front of the chemical formulas (called stoichiometric *coefficients*) and
  - Numbers in the formulas (they appear as subscripts).
- Stoichiometric coefficients give the *ratio* in which the reactants and products exist.
- The subscripts give the ratio in which the atoms are found in the molecule.
  - Example:
    - H_2O means there are <u>two H atoms</u> for each one molecule of water.
    - **2** H_2O means that there are <u>two water molecules</u> present.
- Note: In 2 H_2O there are *four* hydrogen atoms present (two for each water molecule).
- Matter cannot be lost in chemical reactions.
  - Therefore, the products of a chemical reaction have to account for all the atoms present in the reactants.
- Consider the reaction of methane with oxygen.

$$CH_4 + O_2 \dashrightarrow CO_2 + H_2O$$

- Counting *atoms* in the reactants:
  - 1 C;
  - 4 H; and
  - 2 O
- In the products:
  - 1 C;
  - 2H; and
  - 3O
- It appears as though H has been lost and C has been created.
- To balance the equation, we adjust the stoichiometric coefficients:

$$CH_4 + \mathbf{2}\ O_2 \dashrightarrow CO_2 + \mathbf{2}\ H_2O$$

3.2 Patterns of Chemical Reactivity

Using the Periodic Table

- As a consequence of the good ordering of the periodic table, the properties of compounds of elements vary in a systematic manner.
- Example: All the alkali metals (M) react with water as follows:

$$2\,M\,(s) + 2\,H_2O\,(l) \text{ --> } 2\,MOH\,(aq) + H_2\,(g)$$

  - The reactions become more vigorous as we move from Li to Cs
  - Sodium reacts with water to produce an orange flame.
  - Potassium reacts with water to produce a blue flame.
  - The reaction of potassium with water produces so much heat that the hydrogen gas produced usually ignites with a loud pop.

Combustion in Air

- **Combustion reactions** are rapid reactions that produce a flame.
  - Combustion is the burning of a substance in air.
  - Example: Propane combusts to produce carbon dioxide and water:

$$C_3H_8\,(g) + 5\,O_2\,(g) \text{ --> } 3\,CO_2\,(g) + 4\,H_2O\,(l)$$

Combination and Decomposition Reactions

- In **combination reactions** two or more substances react to form one product.
- Combination reactions have more reactants than products.
  - Consider the reaction:

$$2\,Mg\,(s) + O_2\,(g) \text{ --> } 2\,MgO\,(s)$$

    - Since there are fewer products than reactants, the Mg has combined with O_2 to form MgO.
    - Note that the structure of the reactants has changed:
      - Mg consists of closely packed atoms, and O_2 consists of dispersed molecules.
      - MgO consists of a lattice of Mg^{2+} and O^{2-} ions.

- In **decomposition reactions** one substance undergoes a reaction to produce two or more other substances.
- Decomposition reactions have more products than reactants.
  - Consider the reaction that occurs in an automobile air bag:

$$2\,NaN_3\,(s) \text{ --> } 2\,Na\,(s) + 3\,N_2\,(g)$$

  - Since there are more products than reactants, the sodium azide has decomposed into Na metal and N_2 gas.

3.3 Atomic and Molecular Weights

The Atomic Mass Scale

- Consider 100 g of water:
  - Upon decomposition 11.1 g of hydrogen and 88.9 g of oxygen are produced.
  - The mass ratio of O to H in water is 88.9 / 11.1 ~ = 8
  - Therefore, the mass of O is 2 x 8 = 16 times the mass of H
  - If H has a mass of 1, then O has a *relative mass* of 16
  - We can measure atomic masses accurately using a mass spectrometer
  - We know that H-1 has a mass of 1.6735 x 10^{-24} g, and O-16 has a mass of 2.6560 x 10^{-23} g.

- Atomic mass units (amu) are convenient units to use when dealing with extremely small masses of individual atoms.
- 1 amu = 1.66054 x 10^{-24} g and 1 g = 6.02214 x 10^{23} amu
- By definition, the mass of C-12 is exactly 12 amu.

Average Atomic Mass

- We average the masses of isotopes using their masses and relative abundances to give the average atomic mass of an element.
  - Naturally occurring C consists of 98.892% C-12 (12 amu) and 1.108% C-13 (13.00335 amu)
  - The average mass of C is

    (0.98892)(12 amu) + (0.01108)(13.00335) = 12.011 amu

- **Atomic weight** (AW) is also known as average atomic mass.
- Atomic weights are listed on the periodic table.

Formula and Molecular Weights

- **Formula Weight** (FW) is the sum of atomic weights for the atoms shown in the chemical formula.
  - Example: FW (H_2SO_4)
  - 2 AW (H) + AW (s) + 4 AW (O)
  - 2 (1 amu) + 32.1 amu + 4 (16.0 amu)
  - 98.1 amu
- **Molecular weight** is the sum of the atomic weights of the atoms in a molecule as shown in the molecular formula.
  - Example: MW ($C_6H_{12}O_6$)
  - = 6 (12.0 amu) + 12 (1.0 amu) + 6 (16.0 amu)
  - 180.0 amu
- Formula weight of the repeating unit is used for ionic substances.
  - Example: FW (NaCl)
  - = 23.0 amu + 35.5 amu
  - 58.5 amu

Percentage Composition from Formulas

- Percent composition is obtained by dividing the mass contributed by each element (number of atoms times AW) by the formula weight of the compound and multiplying by 100.

The Mass Spectrometer

- Mass spectrometers are pieces of equipment designed to measure atomic and molecular masses accurately.
- The sample is converted to positive ions by collisions with a stream of high-energy electrons upon entering the spectrometer.
- The charged sample is accelerated using an applied voltage.
- The ions are then passed into an evacuated tube through a magnetic field.
- The magnetic field causes the ions to be deflected by different amounts depending on their mass.
- The ions are then detected.

3.4 The Mole

- The mole is a convenient measure of chemical quantities (just as a dozen is a convenient way to measure cooking quantities).
- 1 mole of something is 6.0221421×10^{23} of that thing.
  - This number is called **Avagadro's number.**
  - Thus 1 mole of carbon atoms = 6.0221421×10^{23} carbon atoms.

Molar Mass

- The mass in grams of 1 mole of a substance is said to be the **molar mass** of that substance.
- Molar mass is expressed in units of g/mol (also written $g \cdot mol^{-1}$).
- The mass of 1 mole of C-12 = 12 g
- The molar mass of a molecule is the sum of the molar masses of the atoms
  - Example: The molar mass of N_2 = 2 x (molar mass of N)
- Molar masses for elements are found on the periodic table
- Formula weights are numerically equal to the molar mass.

Interconverting Masses, Moles, and Number of Particles

- Look at units:
  - Mass: g
  - Moles: mol
  - Molar mass: g / mol
  - Number of particles: $6.022 \times 10^{23}\ mol^{-1}$ (Avogadro's number).
  - Note: g/mol x mol = g (i.e. molar mass x moles = mass), and
  - mol x mol^{-1} = a number (i.e. moles x Avogadro's number = molecules)

- To convert between grams and moles, we use the molar mass
- To convert between moles and molecules we use Avogadro's number.

3.5 Empirical Formulas from Analyses

- Recall that the empirical formula gives the *relative* number of atoms in the molecule.
- Finding the empirical formula from mass percent data:
  - We start with the mass percent of elements (i.e., empirical data) and calculate a formula
    - Assume we start with 100 g of sample
    - The mass percent then translates as the number of grams of each element in 100 g of sample.
    - From these masses, we calculate the number of moles (using the atomic weight from the periodic table).
    - The lowest whole-numbered ratio of moles is the empirical formula.

- Finding the empirical mass percent of elements from the empirical formula:
  - If we have the empirical formula, we know how many moles of each element are present in 1 mole of the sample.
  - Next, we use molar masses (or atomic weights) to convert to grams of each element.
  - We divide the grams of each element by grams of 1 mole of sample to get the fraction of each element in 1 mole of sample.
  - We multiply each fraction by 100 to convert to a percent.

Molecular Formula from Empirical Formula

- The empirical formula (relative ratio of elements in the molecule) may not be the molecular formula (actual ratio of elements in the molecule).
  - Example: Ascorbic acid (vitamin C) has the empirical formula $C_3H_4O_3$.
  - The molecular formula is $C_6H_8O_6$.
  - To get the molecular formula from the empirical formula, we need to know the molecular weight, MW.
  - The ratio of molecular weight (MW) to formula weight (FW) of the empirical formula must be a whole number.

Combustion Analysis

- Empirical formulas are routinely determined by combustion analysis.
- A sample containing C, H, and O is combusted in excess oxygen to produce CO_2 and H_2O.
- The amount of CO_2 gives the amount of C originally present in the sample.
- The amount of H_2O gives the amount of H originally present in the sample.
  - Watch stoichiometry: 1 mol H_2O contains 2 mol H
- The amount of O originally present in the sample is given by the difference in the amount of sample and the amount of C and H accounted for.
- More complicated methods can be used to quantify the amounts of other elements present, but they rely on analogous methods.

3.6 Quantitative Information from Balanced Equations

- The coefficients in a balanced chemical equation give the relative numbers of molecules (or formula units) involved in the reaction.
- We can interpret this equation as the *number of moles of reactant* that are required to give the *number of moles of product*.
  - A *stoichiometric ratio* is the ratio of the number of moles of one reactant or product to the number of moles of another reactant or product.
- It is important to realize that the stoichiometric ratios are the ideal proportions in which reactants are needed to form products.
- The real ratio of reactants and products present in the laboratory needs to be measured (in grams and converted to moles).
- The number of grams of a reactant cannot be *directly* related to the number of grams of a product.
  - To get grams of product from grams of reactant.
  - Convert grams of reactant to moles of reactant (use molar mass).
  - Convert moles of reactant to moles of desired product (use the stoichiometric ratio from the balanced chemical equation).
  - Convert moles back into grams for desired product (use molar mass).

3.7 Limiting Reactants

- It is not necessary to have all reactants present in stoichiometric amounts.
- Often, one or more reactants are present in excess.
- Therefore, at the end of the reaction, those reactants present in excess will still be in the reaction mixture.
- The one or more reactants that are completely consumed are called the **limiting reactants**.
- Consider 10 H_2 molecules mixed with 7 O_2 molecules that react to form water.
  - The balanced chemical equation tells us that the stoichiometric ratio of H_2 to O_2 is 2 to 1.
  - This means that our 10 H_2 molecules requires 5 O_2 molecules (2:1)
  - Since we have 7 O_2 molecules, our reaction is *limited* by the amount of H_2 we have (the O_2 present in excess).
  - So, all 10 H_2 molecules can (and do) react with 5 of the O_2 molecules to produce 10 H_2O molecules.
  - At the end of the reaction, 2 O_2 molecules remain unreacted.

Theoretical Yield

- The amount of product predicted from stoichiometry taking into account limiting reagents is called the **theoretical yield**.
- The **percent yield** relates the actual yield (amount of material recovered in the laboratory) to the theoretical yield:

$$Percent\ yield = \frac{actual\ yield}{theoretical\ yield} x\ 100$$