Chapter 3. Stoichiometry: Calculations with Chemical Formulas and Equations

Lecture Outline

3.1 Chemical Equations

- The quantitative nature of chemical formulas and reactions is called **stoichiometry**.
- Lavoisier observed that mass is conserved in a chemical reaction.
    - This observation is known as the l**aw of conservation of mass**.
- **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):

$$2H_2 + O_2 \rightarrow 2H_2O$$

- 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 $2H_2O$ there are *four* hydrogen atoms present (two for each water molecule).

Balancing Equations

- Matter cannot be lost in any chemical reaction.
    - Therefore, the products of a chemical reaction have to account for all the atoms present in the reactants--we must *balance* the chemical equation.
    - When balancing a chemical equation we adjust the stoichiometric coefficients in front of chemical formulas.
        - Subscripts in a formula are *never* changed when balancing an equation.
        - Example: the reaction of methane with oxygen:

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

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

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

Indicating the States of Reactants and Products

- The physical state of each reactant and product may be added to the equation:

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

- Reaction conditions occasionally appear above or below the reaction arrow (e.g., "∞" is often used to indicate the addition of heat).

3.2 Some Simple Patterns of Chemical Reactivity

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:

$$2Mg(s) + O_2(g) \rightarrow 2MgO(s)$$

    - 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:

$$2NaN_3(s) \rightarrow 2Na(s) + 3N_2(g)$$

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

Combustion in Air

- **Combustion reactions** are rapid reactions that produce a flame.
  - Most combustion reactions involve the reaction of $O_2(g)$ from air.
  - Example: combustion of a hydrocarbon (propane) to produce carbon dioxide and water.

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$

3.3 Formula Weights

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)
    - = 2AW(H) + AW(S) + 4AW(O)
    - = 2(1.0 amu) + 32.1 amu + 4(16.0 amu)
    - = 98.1 amu.
- **Molecular weight** (MW) 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 (*formula unit)* is used for ionic substances.
  - Example: FW (NaCl)
    - = 23.0 amu + 35.5 amu
    - = 58.5 amu.

Percentage Composition from Formulas

- *Percentage 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.

$$\%\ \text{element} = \frac{(\text{number of atoms of that element})(\text{atomic weight of element})(100)}{(\text{formula weight of compound})}$$

3.4 Avogadro's Number and The Mole

- The **mole** (abbreviated "mol") is a convenient measure of chemical quantities.
- 1 mole of something = 6.0221421 x 10^{23} of that thing.
  - This number is called **Avogadro's number**.
  - Thus, 1 mole of carbon atoms = 6.0221421 x 10^{23} carbon atoms.
- Experimentally, 1 mole of ^{12}C has a mass of 12 g.

Molar Mass

- The mass in grams of 1 mole of substance is said to be the **molar mass** of that substance. Molar mass has units of g/mol (also written $g \mid mol^{-1}$).
- The mass of 1 mole of ^{12}C = 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.
- The formula weight (in amu) is numerically equal to the molar mass (in g/mol).

Interconverting Masses and Moles

- Look at units:
  - Mass: g
  - Moles: mol
  - Molar mass: g/mol
- To convert between grams and moles, we use the molar mass.

Interconverting Masses and Number of Particles

- Units:
  - Number of particles: 6.022 x 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 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 of each element in the molecule.
- Finding 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, the number of moles can be calculated (using the atomic weights from the periodic table).
  - The lowest whole-number 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 is present in one mole of the sample.
  - Then we use molar masses (or atomic weights) to convert to grams of each element.
  - We divide the number of grams of each element by the number of grams of 1 mole of sample to get the fraction of each element in 1 mole of sample.
  - 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 the stoichiometry: 1 mol H_2O contains 2 mol H.
- The amount of O originally present in the sample is given by the difference between 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.
- The stoichiometric coefficients in the balanced equation may be interpreted as:
  - the relative numbers of molecules or formula units involved in the reaction or
  - the relative numbers of moles involved in the reaction.
- The molar quantities indicated by the coefficients in a balanced equation are called *stoichiometrically equivalent quantities*.
- Stoichiometric relations or ratios may be used to convert between quantities of reactants and products in a reaction.
- It is important to realize that the stoichiometric ratios are the ideal proportions in which reactants are needed to form products.
- The number of grams of reactant cannot be *directly* related to the number of grams of product.
  - To get grams of product from grams of reactant:
    - convert grams of reactant to moles of reactant (use molar mass),
    - convert moles of one reactant to moles of other reactants and products (use the stoichiometric ratio from the balanced chemical equation), and then
    - 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 is present in excess.
- Therefore, at the end of 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 or limiting reagents**.
  - Reactants present in excess are called *excess reactants* or *excess reagents*.
- Consider 10 H_2 molecules mixed with 7 O_2 molecules to form water.
  - The balanced chemical equation tells us that the stoichiometric ratio of H_2 to O_2 is 2 to 1:

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

  - This means that our 10 H_2 molecules require 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 is present in excess).

- So, all 10 H_2 molecules can (and do) react with 5 of the O_2 molecules producing 10 H_2O molecules.
- At the end of the reaction, 2 O_2 molecules remain unreacted.

Theoretical Yields

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

$$\text{Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$