Ch 3. Stoichiometry: Calculations w Chemical Formulas & Eqns

Common Student Misconceptions

- Students who have good high school backgrounds find this chapter quite easy. Those who have poor high school backgrounds find this chapter extremely difficult. Very few students have heard the term *stoichiometry* and can be intimidated by the language of chemistry.
- Students have a problem with differentiating between the subscript in a chemical formula and the coefficient of the formula.
- Balancing equations requires some trial and error. Algorithm-loving students find this uncomfortable.
- Many students will be unfamiliar with "National Mole Day" (i.e., that 6:02 AM on October 23 is the start of National Mole Day).
- Some students cannot distinguish between the number of moles actually manipulated in the laboratory versus the number of moles required by stoichiometry.
- Students do not appreciate that the coefficients in an empirical formula are not exact whole numbers because of experimental or round-off errors. In general, students have problems with the existence of experimental error.
- The concept of limiting reagents is one of the most difficult for beginning students. Part of the problem is that students do not understand the difference between the amount of material present in the laboratory (or given in the problem) and the number of moles required by stoichiometry.
- Students do not understand that the reagent that gives the smallest amount of product is the limiting reagent. They need much numerical practice at this concept. The use of analogies is often quite helpful.
- Students are often quite happy with a percent yield in excess of 100%.

Textbook 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., "Δ" 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 (AW) for the atoms shown in a 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 AWs of the atoms in a ***molecule*** as shown in a 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 always 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.

$$\% \text{ element} = \frac{(\text{number of atoms of that element})(\text{AW of element})(100)}{\text{FW of compound}}$$

Sample Problem: Ethane – molecular formula C_2H_6

3.4 Avogadro's Number and The Mole

- The **mole** (abbreviated "mol") is a convenient measure of chemical quantities.
- 1 mole of something = 6.0221421×10^{23} of that thing.
  - This number is called **Avogadro's number**.
  - Thus, 1 mole of carbon atoms = 6.0221421×10^{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 $g \cdot mol^{-1}$).
- 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: $6.022 \times 10^{23}\ mol^{-1}$ (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 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.

Sample Problem: The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

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).

Sample Problem: How many grams of water are produced in the oxidation of 1.00 g of glucose, $C_6H_{12}O_6$?

$$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$$

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.

Sample Problem: The most important commercial process for converting N_2 from the air into nitrogen-containing compounds is based on the reaction of N_2 and H_2 to form ammonia (NH_3):

$$N_2(g) + 3\,H_2(g) \longrightarrow 2\,NH_3(g)$$

How many moles of NH_3 can be formed from 3.0 mol of N_2 and 6.0 mol of H_2?

Theoretical Yield

- The amount of product predicted from stoichiometry, taking into account limiting reagents, is called the **theoretical yield**. This is what you calculated above!

- This is often different from the *actual yield* -- the amount of product actually obtained in the lab.
- The **percent yield** relates the actual yield (amount of material recovered in the laboratory) to the theoretical, calculated yield:

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