Chapter 5: Calculations and the Chemical Equation

5.1 The Mole Concept and Atoms

- **The Mole and Avogadro’s Number**
  - Atomic mass unit (amu) - unit of measure for the mass of atoms.
  - Carbon-12 assigned the mass of exactly 12 amu.
  - 1 amu = 1.66 x 10^{-24} g
  - Periodic table gives atomic weights in amu.
  - Chemists usually work with much larger quantities.
    - It is more convenient to work with grams than amu.
  - To make the connection we must define the **mole**.
  - The mole is abbreviated mol.
  - Avogadro’s number = 1 mol of atoms = 6.022 x 10^{23} atoms of an element.
  - A mole is simply a unit that defines an amount of something.
    - Just as a dozen defines 12.
    - Just as a gross defines 144.
  - **Molar mass** - The mass in grams of 1 mole of atoms.
  - What is the molar mass of carbon? 12.01 g/mol
  - This means if you counted out a mole of Carbon atoms (i.e., 6.022 x 10^{23} of them) they would have a mass of 12.01 g.
  - The average mass of one atom of an element in amu is numerically equivalent to the mass of one mole of an element expressed in grams.
    - That is, 1 atom F is 19.00 amu and 1 mole of F is 19.00 g. Or,
    - 19.00 amu/atom F and 19.00 g/mole F.

5.2 Compounds

- **The Chemical Formula**
  - Chemical Formula - a combination of symbols of the various elements that make up the compound.
  - **Formula unit** - the smallest collection of atoms that provide two important pieces of information.
    - The identity of the atoms and
    - The relative number of each type of atom.
  - Let’s look closely at the following formulas:
    - H$_2$O, NaCl, Fe(CN)$_3$, (NH$_4$)$_3$PO$_4$, CuSO$_4$.5H$_2$O
    - This is an example of a hydrate - compounds containing one or more water molecules as an integral part of their structure.

5.3 The Mole Concept Applied to Compounds

- **Formula weight** - the sum of the atomic weights of all atoms in the compound, as represented by its formula.
  - Expressed in amu.
  - Molar mass applies to compounds also.
- **What is the formula weight of H$_2$O?**
  - 16.00 amu + 2(1.008 amu) = 18.02 amu
- **What is the molar mass of H$_2$O?**
• 18.02 g/mol H₂O
  - When calculating the formula weight (or molar mass of an ionic compound, use the smallest unit of the crystal)

5.4 The Chemical Equation and the Information It Conveys
- A Recipe For Chemical Change
  - **Chemical Equation** - shorthand notation of a chemical reaction.
  - **Reactants** - (starting materials) - the substances that undergo change in the reaction.
  - **Products** - substances produced by the reaction.
  - **Law of Conservation of Mass** - matter cannot be either gained or lost in the process of a chemical reaction.
    - The total mass of products must equal the total mass of the reactants.
  - We know that a chemical equation represents a chemical change. The following is evidence for a reaction:
    - Release of a gas.
      - CO₂ is released when acid is placed in a solution containing CO₃²⁻ ions.
      - H₂ is released when Na is placed in water.
    - Formation of a solid (precipitate.)
      - A solution containing Ag⁺ ions is mixed with a solution containing Cl⁻ ions.
    - Heat is produced or absorbed (temperature changes)
      - Acid and base are mixed together
    - The color changes
    - Light is absorbed or emitted
    - Changes in the way the substances behave in an electrical or magnetic field
    - Changes in electrical properties.

5.5 Balancing Chemical Equations
- Consider the following reaction:
  - **hydrogen reacts with oxygen to produce water**
- Write the above reaction as a chemical equation.
- You probably wrote the following:
  - H₂ + O₂ → H₂O
- Don’t forget the diatomic elements.
- Is the law of conservation of mass obeyed as written? NO!
- Balancing chemical equations uses **coefficients** to ensure that the law of conservation of mass is obeyed.
- You may not change subscripts!
- **WRONG**: H₂ + O₂ → H₂O₂

5.6 Calculations Using the Chemical Equation
- We will learn in this section to calculate quantities of reactants and products in a chemical reaction.
- Need a **balanced** chemical equation for the reaction of interest.
- Keep in mind that the **coefficients** represent the number of **moles** of each substance in the equation.
Theoretical and Percent Yield

- **Theoretical yield** - the maximum amount of product that can be produced
  - Pencil and paper yield
- **Actual yield** - the amount produced when the reaction is performed
  - Laboratory yield
- **Percent yield**: actual yield divided by theoretical yield X 100