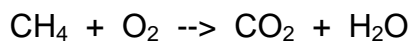


### 3.1 Chemical Equations

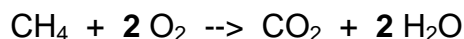
- Lavoisier observed that mass is conserved in a chemical reaction.
  - This observation is known as the **law of conservation of mass**.
- The quantitative nature of chemical formulas and reactions is called **stoichiometry**.
- **Chemical equations** give a description of a chemical reaction.
- **There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



- 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:
    - $\text{H}_2\text{O}$  means there are two H atoms for each one molecule of water.
    - $2 \text{H}_2\text{O}$  means that there are two water molecules present.
- Note: In  $2 \text{H}_2\text{O}$  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.



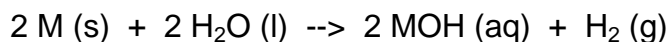
- Counting *atoms* in the reactants:
  - 1 C;
  - 4 H; and
  - 2 O
- In the products:
  - 1 C;
  - 2H; and
  - 3O
- It appears as though H has been lost and C has been created.
- To balance the equation, we adjust the stoichiometric coefficients:



## 3.2 Patterns of Chemical Reactivity

### Using the Periodic Table

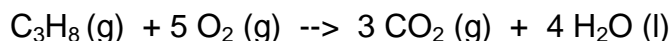
- As a consequence of the good ordering of the periodic table, the properties of compounds of elements vary in a systematic manner.
- Example: All the alkali metals (M) react with water as follows:



- 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.

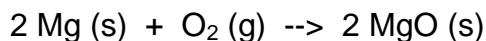
### Combustion in Air

- **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:



### 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:



- Since there are fewer products than reactants, the Mg has combined with O<sub>2</sub> to form MgO.
- Note that the structure of the reactants has changed:
  - Mg consists of closely packed atoms, and O<sub>2</sub> consists of dispersed molecules.
  - MgO consists of a lattice of Mg<sup>2+</sup> and O<sup>2-</sup> 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:
$$2 \text{ NaN}_3 \text{ (s)} \rightarrow 2 \text{ Na (s)} + 3 \text{ N}_2 \text{ (g)}$$
  - Since there are more products than reactants, the sodium azide has decomposed into Na metal and N<sub>2</sub> 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  $88.9 / 11.1 \sim 8$
  - Therefore, the mass of O is  $2 \times 8 = 16$  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  $1.6735 \times 10^{-24}$  g, and O-16 has a mass of  $2.6560 \times 10^{-23}$  g.
- Atomic mass units (amu) are convenient units to use when dealing with extremely small masses of individual atoms.
- $1 \text{ amu} = 1.66054 \times 10^{-24} \text{ g}$  and  $1 \text{ g} = 6.02214 \times 10^{23} \text{ amu}$
- 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  
 $(0.98892)(12 \text{ amu}) + (0.01108)(13.00335) = 12.011 \text{ amu}$
- **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 ( $\text{H}_2\text{SO}_4$ )
  - $2 \text{ AW (H)} + \text{AW (s)} + 4 \text{ AW (O)}$
  - $2 (1 \text{ amu}) + 32.1 \text{ amu} + 4 (16.0 \text{ amu})$
  - 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 ( $\text{C}_6\text{H}_{12}\text{O}_6$ )
  - $= 6 (12.0 \text{ amu}) + 12 (1.0 \text{ amu}) + 6 (16.0 \text{ amu})$
  - 180.0 amu
- Formula weight of the repeating unit is used for ionic substances.
  - Example: FW (NaCl)
  - $= 23.0 \text{ amu} + 35.5 \text{ amu}$
  - 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  $6.0221421 \times 10^{23}$  of that thing.
  - This number is called **Avogadro's number**.
  - Thus 1 mole of carbon atoms =  $6.0221421 \times 10^{23}$  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  $\text{g} \cdot \text{mol}^{-1}$ ).
- 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  $\text{N}_2$  = 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:  $6.022 \times 10^{23} \text{ mol}^{-1}$  (Avogadro's number).
  - Note:  $\text{g/mol} \times \text{mol} = \text{g}$  (i.e. molar mass x moles = mass), and
  - $\text{mol} \times \text{mol}^{-1} = \text{a number}$  (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<sub>2</sub> molecules mixed with 7 O<sub>2</sub> molecules that react to form water.
  - The balanced chemical equation tells us that the stoichiometric ratio of H<sub>2</sub> to O<sub>2</sub> is 2 to 1.
  - This means that our 10 H<sub>2</sub> molecules requires 5 O<sub>2</sub> molecules (2:1)
  - Since we have 7 O<sub>2</sub> molecules, our reaction is *limited* by the amount of H<sub>2</sub> we have (the O<sub>2</sub> present in excess).
  - So, all 10 H<sub>2</sub> molecules can (and do) react with 5 of the O<sub>2</sub> molecules to produce 10 H<sub>2</sub>O molecules.
  - At the end of the reaction, 2 O<sub>2</sub> 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:

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