9.1.1 CHEMICAL EQUATIONS AND STOICHIOMETRY

Work directly from Zumdahl (Chapter 3). Work through exercises as required, then summarise the essentials of the section when complete.

A chemical equation is a shorthand method of describing a chemical reaction, and stoichiometry deals with the amounts of substances consumed and/or produced in such a reaction.

9.1.1.1 Atomic Mass

We count atoms by measuring the mass of a sample, and we relate this mass to the number of atoms present using the average atomic mass (or atomic weight) of the atom in question. The modern system of atomic masses, instituted in 1961, is based on ^{12}C ("carbon twelve") as the standard. In this system, *^{12}C is assigned a mass of exactly 12 atomic mass units* (**amu**), and the masses of all other atoms are given relative to this standard.

In spite of this, we will note that the atomic mass of carbon is more often listed as 12.01. The reason for this apparent discrepancy is that carbon found on Earth (natural carbon) is a mixture of the isotopes ^{12}C, ^{13}C and ^{14}C. All three isotopes have six protons, but they have six, seven and eight neutrons, respectively. Because natural carbon is a mixture of isotopes, the atomic mass we use for carbon is an average value, 98.89% ^{12}C and 1.11% ^{13}C (at this level of precision, the amount of ^{14}C present is negligibly small) reflecting the average of the isotopes of which it is composed.

The average atomic mass of any element reflects the isotopic composition of a natural sample of that element.

9.1.1.2 The Mole

Because samples of matter typically contain so many atoms, a unit of measure called the **mole** has been established for use in counting atoms. One mole (abbreviated mol) is defined as being equal to the number of carbon atoms in exactly 12g of pure ^{12}C, that being 6.022×10^{23} units of a substance. This number is known as **Avogadro's number** (**N_A**), after the Italian scientist Amedeo Avogadro (1776 – 1856).

The mass of one mole of an element is equal to its atomic mass in grams.

Sample exercises 3.2 – 3.5

9.1.1.3 Molar Mass

The **molar mass**, also known as the **molecular weight**, of a substance is the mass in grams of one mole of the compound. It is derived by adding up the respective atomic masses of the component atoms. For example, the molar mass, or molecular weight of ethanol (C_2H_5OH) is calculated as follows:

Mass of 2 mol **C**	=	2 x 12.01 g	=	24.02 g
Mass of 6 mol **H**	=	6 x 1.008 g	=	6.048 g
Mass of 1 mol **O**			=	16.00 g
Mass of 1 mol C_2H_5OH			=	46.07 g

Sample exercises 3.6 – 3.8

9.1.1.4 Percent Composition of Compounds

The are two common ways of describing the composition of a compound: in terms of the numbers of its constituent atoms (*i.e.* its molecular formula) and in terms of the percentages (by mass) of its elements.

The **mass percent** of each element in a compound is given by the equation:

$$\text{Mass percent} = \frac{\text{mass of element in 1 mole of substance}}{\text{mass of 1 mole of substance}} \times 100\%$$

Thus, continuing with the example of ethanol ($\mathbf{C_2H_5OH}$), the mass percent (or weight percent) of carbon in ethanol is given by:

$$\text{Mass percent of } \mathbf{C} = \frac{\text{mass of } \mathbf{C} \text{ in 1 mol } \mathbf{C_2H_5OH}}{\text{mass of 1 mol } \mathbf{C_2H_5OH}} \times 100\%$$

$$= \frac{24.02 \text{ g}}{46.07 \text{ g}} \times 100\% = 52.14\%$$

The mass percent of hydrogen and oxygen in ethanol are obtained in a similar manner:

$$\text{Mass percent of } \mathbf{H} = \frac{\text{mass of } \mathbf{H} \text{ in 1 mol } \mathbf{C_2H_5OH}}{\text{mass of 1 mol } \mathbf{C_2H_5OH}} \times 100\%$$

$$= \frac{6.048 \text{ g}}{46.07 \text{ g}} \times 100\% = 13.13\%$$

$$\text{Mass percent of } \mathbf{O} = \frac{\text{mass of } \mathbf{O} \text{ in 1 mol } \mathbf{C_2H_5OH}}{\text{mass of 1 mol } \mathbf{C_2H_5OH}} \times 100\%$$

$$= \frac{16.00 \text{ g}}{46.07 \text{ g}} \times 100\% = 34.73\%$$

Sample exercises 3.9 & 3.10

9.1.1.5 Determining the Formula of a Compound

9.1.1.5.1 Empirical Formula

The **empirical formula** is the simplest whole number ratio of the various types of atoms in a compound. It can be determined from the respective mass percentages of the individual elements in a compound.

Empirical Formula Determination

1 Since mass percentage gives the number of grams of a particular element per 100 grams of compound, base the calculation on 100 grams of compound. Each percent will then represent the mass in grams of that element;

2 Determine the number of moles of each element present in 100 grams of compound using the atomic masses of the elements present;

3 Divide each value of the number of moles by the smallest of the values. If each resulting number is a whole number (after appropriate rounding), these numbers represent the subscripts of the elements in the empirical formula;

4 If the numbers obtained in the previous step are not whole numbers, multiply each number by an integer so that the results are all whole numbers.

9.1.1.5.2 Molecular Formula

Molecular Formula = **(Empirical Formula)$_{n}$**
where **n** is an integer

For molecular substances:
The formula of the constituent atoms
Always an integer multiple of the empirical formula

For ionic substances:
The same as the empirical formula

To determine the molecular formula, we need to know both the empirical formula and the molar mass of the compound in question.

Sample exercises 3.11 – 3.13

Molecular Formula Determination

Method 1

1 Obtain the empirical formula;

2 Compute the mass corresponding to the empirical formula;

3 Calculate the ratio:

$$\frac{\text{Molar Mass}}{\text{Empirical formula Mass}}$$

4 The integer from the previous step represents the number of empirical formula units in one molecule. When the empirical formula subscripts are multiplied by this integer, the molecular formula results. This procedure is summarised by the equation:

$$\text{Molecular Formula} = (\text{Empirical Formula}) \times \frac{\text{Molar Mass}}{\text{Empirical formula Mass}}$$

Method 2

1. Using the mass percentages and the molar mass, determine the mass of each element present in one mole of compound;
2. Determine the number of moles of each element present in one mole of compound;
3. The integers from the previous step represent the subscripts in the molecular formula

9.1.1.6 Chemical Equations[M38]

9.1.1.6.1 Chemical Reactions

We have seen that decomposition is the breaking down of a substance into its components—either elements or less complex substances—and that synthesis is the process by which compounds, or more complex substances, are created from elements or less complex substances. In both cases, reactants are turned into products, and atoms are neither created nor destroyed—all of the atoms present in the reactants are also present in the products. Chemists use a shorthand method to describe these processes, and indeed chemical reactions in general.

9.1.1.6.2 The Meaning of a Chemical Equation

The symbols or molecular formulae for the elements and/or compounds involved are used to write a **chemical equation** as a summary of a chemical reaction. In the chemical equation the **reactant(s)** are written on the left hand side of an arrow and the **product(s)** on the right hand side, as illustrated in the simple equation for the formation of water (H_2O) from hydrogen (H_2) and oxygen (O_2).

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

The (electrolytic) decomposition of water into its constituents is simply the reverse of this reaction:

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

Where relevant, the physical states of the substances can be indicated by the subscripts *s*, *l* or *g*.

$$2HgO(s) \rightarrow 2Hg(l) + O_2(g)$$

When balanced, a chemical equation also identifies the relative numbers of reactant and product molecules or ions involved in the reaction.

9.1.1.6.3 Valency and Formula Writing

Used in its most general sense, **valency** is a measure of the **combining power** of an element. While there are several different definitions of valency, it will serve our needs to define it as being equal to the number of hydrogen atoms that will combine with or displace one atom of the element. In general, except for the transition elements, this is also the lesser of the number of electrons required to fill or empty the outermost electron shell. Where electron movement empties the outer shell, the valency is taken to be positive, where it fills the outer shell the valency is taken to be negative. These valency electrons are given up to or are received from other atoms to create **ionic bonds**, or they are shared with other atoms to form **covalent bonds**.

Thus, sodium, which loses one electron to form the Na^+ ion, has a valency of +**1**, while chlorine, which gains one electron to form the Cl^- ion, has a valency of -**1**. Similarly, calcium has a valency of +**2**, losing two electrons to empty its out electron shell and form the Ca^{2+} ion, and oxygen [most often] has a valency of -**2**, gaining two electrons to fill its outer shell. Carbon, which generally forms covalent bonds, can have a valency of either +**4** or -**4**, depending on the element(s) with which it combines—*cf.* methane (CH_4) and carbon tetrachloride (CCl_4).

The **name of a compound** often comprises the **names of the elements** that make up the compound. The valency of an element, if it is variable (as is often the case for transition elements), is included in the name as well as the number of atoms present in the formula for the compound. Thus, as we have just seen, carbon tetrachloride (CCl_4) is the compound formed by combining a single carbon atom with four chlorine atoms, and iron (II) oxide (FeO) and iron (III) oxide (Fe_2O_3) are the distinct compounds formed when iron, in its two different oxidation states, combines with oxygen.

The **formula for a compound** may be written using the symbol for the element to represent one atom of the element and **equating the valencies** of the atoms and ions present in the compound.

The formula represents the **composition of the compound**, and in an equation it represents a mass equal to the molecular weight of the compound.

9.1.1.6.4 Formulae Equations

In a **chemical equation**, formulae for the reactants are written on the left-hand side of an arrow and those of the products on the right-hand side of the arrow. For example, the reaction between potassium chromate and barium nitrate is written as follows:

$$K_2CrO_4(aq) + Ba(NO_3)_2(aq) \longrightarrow BaCrO_4(s) + 2KNO_3(aq)$$

The **equation is balanced** when it is in agreement with the Law of Conservation of Mass, that is, there must be equal numbers of atoms of each element on both sides of the arrow.

9.1.1.6.5 Ionic Equations

Ionic equations must be balanced with respect to both mass and charge. For example, the complete ionic equation for the above reaction is written as follows:

$$2K^+(aq) + CrO_4^{2-}(aq) + Ba^{2+}(aq) + 2NO_3^-(aq) \longrightarrow BaCrO_4(s) + 2K^+(aq) + 2NO_3^-(aq)$$

Positively charged ions are called cations, negatively charged ions are called anions.

9.1.1.6.6 Chemical Calculations

In a **chemical reaction** the **reacting proportions** of the substances involved may be obtained from the **balanced chemical equation** for the reaction. The formula for each compound is taken to represent a mass equal to the molecular weight of the compound.

9.1.1.7 Balancing Chemical Equations

Writing and Balancing the Equation for a Chemical Reaction

1. Determine what reaction is occurring. What are the reactants, the products, and the physical states involved?
2. Write the *unbalanced* equation that summarises the reaction described in Step 1;
3. Balance the equation by inspection, starting with the most complicated molecule(s). Determine what coefficients are necessary so that the same numbers of each type of atom appears on both reactant and product sides. Do not change the identities (formulae) of any of the reactants or products.

Sample exercises 3.14 & 3.15

9.1.1.8 Stoichiometric Calculations

The amounts of reactants consumed and products formed can be determined from the balanced chemical equation.

The limiting reactant is the one consumed first, thus limiting the amount of product that can form.

Calculating Masses of Reactants and Products in Chemical Reactions

1. Balance the equation for the reaction;
2. Convert the known mass of the reactant or product to moles of that substance;
3. Use the balanced equation to set up the appropriate mole ratios;
4. Use the appropriate mole ratios to calculate the number of moles of the desired reactant or product;
5. Convert from moles back to grams if required by the problem.

Sample exercises 3.16 & 3.17

9.1.1.9 Calculations Involving a Limiting Reactant

The theoretical yield is the maximum amount that can be produced from a given amount of the limiting reactant

The actual yield, the amount of product actually obtained, is always less that the theoretical yield

$$\text{Percent yield} = \frac{\text{actual yield (g)}}{\text{theoretical yield (g)}} \times 100\%$$

Sample exercises 3.18 & 3.19

Solving a Stoichiometry Problem Involving Masses of Reactants and Products

1. Write and balance the equation for the reaction;
2. Convert the known masses of substances to moles;
3. Determine which reactant is limiting;
4. Using the amount of the limiting reactant and the appropriate mole ratios, compute the number of moles of the desired product;
5. Convert from moles to grams, using the molar mass.

Exercises

Zumdahl Ch. 3 Exercises 35, 37, 53, 57, 63, 67, 69, 79, 81, 83

References

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Data on and photographs of the chemical elements
http://www.periodictable.com