Stoichiometry and Chemical Calculations

The mole concept

The *mole* unit has been used in counting atoms. The number of carbon atoms in exactly 12 gm of ^{12}C is called Avogadro's number (L) as $6.022x10^{23}$. The magnitude of the this number is very difficult to imagine. One mole is the amount of material which contains Avogadro's number of particles.

Number of moles = weight (gm)/ weight of one mole (gm/mole)

This definition also gives the relationship between the weight of one mole and the gram. In other words, $6.022x10^{23}$atoms of carbon have a mass of 12 g, then

Molar Mass

The **molar mass** of a substance is *the mass in grams of one mole of the compound.* Traditionally, the terms *molecular weight or* molar mass have been used for this quantity.

Percent Composition of Compounds

There are two common ways of describing the composition of a compound: in terms of the numbers of its constituent atoms and the percentages by mass of its elements.

We can obtain the mass percents of the elements from the chemical formula of the compound. It is the mass of each element present in 1 mole of the compound per the total mass of 1 mole of the compound.

Determining the Formula of a Compound

This is most often determined by taking a weighed sample of the compound and either decomposing it into its component elements or reacting it with oxygen to produce substances such as CO_2, H_2O, and N_2 collected and weighed.

Thus, the data are obtained from the results of such analyses provide the mass of each type of element in the compound. Suppose a substance has been prepared that is composed of carbon, hydrogen, and nitrogen. Assuming that all the carbon in the compound is converted to CO_2, To do this, it must be used the fraction (by mass) of carbon in CO_2.

Experimental Determination of Empirical Formulas

The fact that we can determine the empirical formula of a compound if we know the percent composition enables us to identify compounds experimentally. The procedure is as follows. First, chemical analysis tells us the number of grams of each element present in a given amount of a compound. Then, we convert the quantities in grams to number of moles of each element. As a specific example, let us consider the compound ethanol. When ethanol is burned in an apparatus such as carbon dioxide (CO_2) and water (H_2O) are given off.

we can conclude that both carbon (C) and hydrogen (H) were present in ethanol and that oxygen (O) may also be present. (Molecular oxygen was added in the combustion process, but some of the oxygen may also have come from the original ethanol sample.)

The masses of CO_2 and of H_2O produced can be determined by measuring the increase in mass of the CO_2 and H_2O absorbers, respectively. Suppose that in one experiment the combustion of 11.5 g of ethanol produced 22.0 g of CO_2 and 13.5 g of H_2O.

Determination

- Determine the number of moles of each element present in 100 grams of compound
  using the atomic masses of the elements present.
- Divide each value of the number of moles by the smallest of the values. If each resulting number is a whole number, these numbers represent the subscripts of the elements in the empirical formula.
- 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.

Determination of Molecular Formulas

The formula calculated from percent composition by mass is always the empirical formula because the subscripts in the formula are always reduced to the smallest whole numbers. To calculate the actual, molecular formula we must know the approximate molar mass of the compound in addition to its empirical formula. Knowing that the molar mass of a compound must be an integral multiple of the molar mass of its empirical formula.

First Method in determination of molecular formula

- Obtain the empirical formula.
- Calculate the mass corresponding to the empirical formula.
- Calculate the ratio

When the empirical formula subscripts are multiplied by this integer, the molecular formula results. This procedure is summarized by the equation:

$$\text{Molecular formula} = (\text{empirical formula}) \times \frac{\text{molar mass}}{\text{empirical formula mass}}$$

Second method

- Using the mass percentages and the molar mass, determine the mass of each element present in one mole of compound.
- Determine the number of moles of each element present in one mole of compound.

The Chemical equation

The chemical equation for a reaction gives two important types of information: the nature of the reactants and products and the relative numbers of each. The reactants and products in a specific reaction must be identified by experiment. The relative numbers of reactants and products in a reaction are indicated by the *coefficients* in the balanced equation.

A chemical reaction is a mechanical process, it is converted from one physical state to another. For example,

$$2Ag^{+}_{(aq)} + H_2S \rightarrow Ag_2S_{(s)} + 2H^{+}_{(aq)}$$

Balancing Chemical Equations

The identities of products are more difficult to establish. For simple reactions, it is often possible to guess the product(s). For more complicated reactions involving three or more products, it is performed further tests to establish the presence of specific compounds. Once it is identified all the reactants and products and have written the correct formulas for them, we assemble them in the conventional sequence—reactants on the left separated by an arrow from products on the right. The equation written at this point is likely to be unbalanced; that is, the number of each type of atom on one side of the arrow differs from the number on the other side. In general, we can balance a chemical equation by the following steps:

1. Identify all reactants and products and write their correct formulas on the left side and right side of the equation, respectively.

2. Begin balancing the equation by trying different coefficients to make the number of atoms of each element the same on both sides of the equation. It can be changed the coefficients (the numbers preceding the formulas) but not the subscripts (the numbers within formulas). Changing the subscripts would change the identity of the substance. For example, 2NO2 means "two molecules of nitrogen dioxide," but if we double the subscripts, we have N2O4, which is the formula of dinitrogen tetroxide, a completely different compound.

3. First, look for elements that appear only once on each side of the equation with the same number of atoms on each side: The formulas containing these elements must have the same coefficient. Therefore, there is no need to adjust the coefficients of these elements at this point. Next, look for elements that appear only once on each side of the equation but in unequal numbers of atoms. Balance these elements. Finally, balance elements that appear in two or more formulas on the same side of the equation.

4. Check your balanced equation to be sure that you have the same total number of each type of atoms on both sides of the equation arrow.

Stoichiometric Calculations: Amounts of Reactants and Products

Mass Relationships of a Chemical Reaction A chemical equation enables us to predict the amount of product(s) formed, called the yield, knowing how much reactant(s) was (were) used. This information is of great importance for reactions run on the laboratory or industrial scale. In practice, the actual yield is almost always less than that predicted from the equation because of various complications.

The coefficients in chemical equations represent numbers of molecules, not masses of molecules. However, when a reaction is to be run in a laboratory or chemical plant, the amounts of substances needed cannot be determined by counting molecules directly. Counting is always done by weighing. In this section we will see how chemical equations can be used to determine the *masses* of reacting chemicals. To develop the principles for dealing with the stoichiometry of reactions, we will consider the reaction of propane with oxygen to produce carbon dioxide and water. We will consider the question: *"What mass of oxygen will react with 96.1 grams of propane?"* In doing stoichiometry, the first thing we must do is *write the balanced chemical equation* for the reaction. In this case the balanced equation is

A basic question raised in the chemical laboratory is "How much product will be formed from specific amounts of starting materials (reactants)?" Or in some cases, we might ask the reverse question: "How much starting material must be used to obtain a specific amount of product?" To interpret a reaction quantitatively, we need to apply our knowledge of molar masses and the mole concept. Stoichiometry is the quantitativestudy of reactants and products in a chemical reaction. Whether the units given for reactants (or products) are moles, grams, liters (for gases), or some other units, we use moles to calculate the amount of product formed in a reaction. This approach is called the mole method, which means simply that the stoichiometric coefficients in a chemical equation can be interpreted as the number of moles of each substance. For example, the combustion of carbon monoxide in air produces carbon dioxide:

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$

The stoichiometric coefficients show that two molecules of CO react with one molecule of O_2 to form two molecules of CO_2. It follows that the relative numbers of moles are the same as the relative numbers of molecules:

$$\begin{array}{ccccc} 2CO(g) & + & O_2(g) & \longrightarrow & 2CO_2(g) \\ \text{2 molecules} & & \text{1 molecule} & & \text{2 molecules} \\ 2(6.022 \times 10^{23} \text{ molecules}) & & 6.022 \times 10^{23} \text{ molecules} & & 2(6.022 \times 10^{23} \text{ molecules}) \\ \text{2 mol} & & \text{1 mol} & & \text{2 mol} \end{array}$$

Thus, this equation can also be read as "2 moles of carbon monoxide gas combine with 1 mole of oxygen gas to form 2 moles of carbon dioxide gas." In stoichiometric calculations, we say that two moles of CO are equivalent to two moles of CO_2, that is,

$$2 \text{ mol CO} \simeq 2 \text{ mol } CO_2$$

where the symbol ∞ means "stoichiometrically equivalent to" or simply "equivalent to." The mole ratio between CO and CO_2 is 2:2 or 1:1, meaning that if 10 moles of CO are reacted, 10 moles of CO2 will be produced. Likewise, if 0.20 mole of CO is reacted, 0.20 mole of CO_2 will be formed. This relationship enables us to write the conversion factors

$$\frac{2 \text{ mol CO}}{2 \text{ mol CO}_2} \quad \text{and} \quad \frac{2 \text{ mol CO}_2}{2 \text{ mol CO}}$$

Let's consider a simple example in which 4.8 moles of CO react completely with O_2 to form CO_2. To calculate the amount of CO_2 produced in moles, we use the conversion factor that has CO in the denominator and write

$$\begin{aligned} \text{moles of CO}_2 \text{ producted} &= 4.8 \cancel{\text{mol CO}} \times \frac{2 \text{ mol CO}_2}{2 \cancel{\text{mol CO}}} \\ &= 4.8 \text{ mol CO}_2 \end{aligned}$$

Now suppose 10.7 g of CO react completely with O_2 to form CO_2. How many grams of CO_2 will be formed? To do this calculation, we note that the link between CO and CO_2 is the mole ratio from the balanced equation. So we need to first convert grams of CO to moles of CO, then to moles of CO_2, and finally to grams of CO_2. The conversion steps are

$$\text{grams of CO} \longrightarrow \text{moles of CO} \longrightarrow \text{moles of CO}_2 \longrightarrow \text{grams of CO}_2$$

First we convert 10.7 g of CO to number of moles of CO, using the molar mass of CO as the conversion factor:

$$\begin{aligned} \text{moles of CO} &= 10.7 \cancel{\text{g CO}} \times \frac{1 \text{ mol CO}}{28.01 \cancel{\text{g CO}}} \\ &= 0.382 \text{ mol CO} \end{aligned}$$

Next we calculate the number of moles of CO_2 produced:

$$\text{moles of } CO_2 = 0.382 \ \cancel{\text{mol CO}} \times \frac{2 \text{ mol } CO_2}{2 \ \cancel{\text{mol CO}}}$$
$$= 0.382 \text{ mol } CO_2$$

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.

Calculations Involving a Limiting Reactant

When chemicals are mixed together to undergo a reaction, they are often mixed in **stoichiometric quantities,** that is, in exactly the correct amounts so that all reactants "run out" (are used up) at the same time. To clarify this concept, let's consider the production of hydrogen for use in the manufacture of ammonia by the **Haber process.** Ammonia, a very important fertilizer itself and a starting material for other fertilizers, is made by combining nitrogen (from the air) with hydrogen according to the equation

When a chemist carries out a reaction, the reactants are usually not present in exact stoichiometric amounts, that is, in the proportions indicated by the balanced equation. Because the goal of a reaction is to produce the maximum quantity of a useful compound from the starting materials, frequently a large excess of one reactant is supplied to ensure that the more expensive reactant is completely converted to the desired product. Consequently, some reactant will be left over at the end of the reaction. The reactant used up first in a reaction is called the limiting reagent, because the maximum amount of product formed depends on how much of this reactant was originally present. When this reactant is used up, no more product can be formed. Excess reagents are the reactants present in quantities greater than necessary to react with the quantity of the limiting reagent.

The concept of the limiting reagent is analogous to the relationship between men and women in a dance contest at a club. If there are 14 men and only 9 women, then only 9 female/male pairs can compete. Five men will be left without partners. The number of women thus limits the number of men that can dance in the contest, and there is an excess of men.

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.

Reaction Yield

The amount of limiting reagent present at the start of a reaction determines the theoretical yield of the reaction, that is, the amount of product that would result if all the limiting reagent reacted. The theoretical yield, then, is the maximum obtainable yield, predicted by the balanced equation. In practice, the actual yield, or the amount of product actually obtained from a reaction, is almost always less than the theoretical yield. There are many reasons for the difference between actual and theoretical yields. For instance, many reactions are reversible, and so they do not proceed 100 percent from left to right. Even when a reaction is 100 percent complete, it may be difficult to recover all of the product from the reaction medium. Some reactions are complex in the sense that the products formed may react further among themselves or with the reactants to form still other products. These additional reactions will reduce the yield of the first reaction.

To determine how efficient a given reaction is, chemists often figure the percent yield, which describes the proportion of the actual yield to the theoretical yield. It is calculated as follows:

$$\%\ \text{yield} = \frac{\text{actual yield}}{\text{theoritical yield}} \times 100\%$$

Percent yields may range from a fraction of 1 percent to 100 percent. Chemists strive to maximize the percent yield in a reaction. Factors that can affect the percent yield include temperature and pressure. We will study these effects later.