CHAPTER 1 – STOICHIOMETRY

Introduction

Chemistry – A Molecular Science (CAMS), the first half of this two-course sequence, stressed bonding, structure, and reactivity. The material was qualitative and stressed several types of reactions and the factors that affected their relative extents of reaction. However, as the title of this text suggests, chemistry is also a quantitative science. Chemists must not only predict the products of a reaction, they must also predict the amount of product that can be expected, and the amount of waste that must be removed. They also need to know how much energy is required or how much heat is generated by a reaction. They must also understand how the reaction occurs so that they can optimize the reaction conditions. These are the types of problems addressed in this text.

We begin our study of the quantitative aspects of chemistry with stoichiometry, the science that deals with the quantitative relationships between the elements in a compound (substance stoichiometry) and between the substances in a chemical reaction (reaction stoichiometry). It is the topic of this first chapter because a thorough knowledge of stoichiometry is vital to an understanding of the material presented in this course. Understanding how quantitative data and results are presented is also important, so you should review Appendix A, Reporting Quantitative Measurements and Results, for a treatment of precision, significant figures, and rounding errors. Finally, we will set up many problems using the factor label method, so please review Appendix B, The Factor Label Method, for a discussion of this procedure.

1.1 Mass and Moles

Introduction

Chemists use chemical equations to design possible routes to desired molecules and to discuss chemical processes. However, the individual molecules represented in the equations are far too small to be seen, so chemists must use a very large number of molecules in their reactions in order that the reactants and products can be observed. Indeed, the number of molecules required to make a visible sample is staggering. Consider that 1 μL of water—about $1/50^{\text{th}}$ of a drop—contains about 100,000,000,000,000,000 or 10^{17} molecules and a typical reaction in the laboratory involves thousands of times that number. Such large numbers are cumbersome, so scientists use a more convenient unit when discussing numbers of molecules. The unit is the mole, the topic of this section.

Objectives

- Convert between numbers of moles and numbers of particles with Avogadro's number.
- Convert between mass and moles with molar mass.
- Convert between the pressure, volume, and temperature of a gas and the number of moles with the ideal gas law.

1.1-1. Avogadro's Number

Avogadro's number, which is given below, is simply the number of items in a mole, so it also defines the ***mole***, which is simply Avogadro's number of items.

$$N_{\text{A}} = 6.0221 \times 10^{23}\text{mol}^{-1} \qquad \text{Avogadro's Number}$$

A mole is used to indicate a number of items just as a dozen is used to indicate a number of eggs. Since Avodagro's number is so large, the mole is used only for the number of atoms or molecules, but it can be used for any item. For example, it is estimated that there are about 10^{23}–10^{24} stars in the universe, which is 1–10 moles. Converting from moles to atoms or molecules is done in the same way as converting dozens to items.
1.5 doz = (1.5 doz)(12 items/doz) = 18 items and 1.5 mol = (1.5 mol)(6.0 × 10^{23} atoms/mol) = 9.0 × 10^{23} atoms. The mole is used simply because it is much easier to discuss the number of atoms in moles than it is as individual items. 0.10 mol H_2O is a much more convenient expression than 6.0 × 10^{22} H_2O molecules.

1.1-2. Molar Mass (M_m)

Chemists need to be able to readily prepare mixtures of reactants that have the correct atom or molecule ratios for reaction, but they certainly cannot count such large numbers. Instead, they use other more easily determined properties that are related to the numbers of atoms and/or molecules. The first such method we examine is mass. Mass can be used to "count" atoms and molecules because a mole is the number of atoms present in one gram atomic weight (the atomic weight expressed in grams) of any atom or in one gram molecular weight of any molecule. Thus, the mass of a mole of any substance, which is known as its ***molar mass*** (M_m), equals its atomic or molecular weight expressed in grams. For example, the atomic weight of Mg is 24.3, so its molar mass 24.3 g/mol, and the molecular weight of CO_2 is 44.0, so its molar mass is 44.0 g/mol. Thus, molar mass allows us to quickly convert a mass into a number of moles or a number of moles into a mass. Chemists use this fact to quickly "count" the number of moles of substance by simply weighing it.

Mole ↔ mass conversions are most easily done with the factor label method. It uses the units of the given quantity and those of the conversion factors to assure the proper operations are performed. To use this method, arrange the factors so that the denominator of each factor cancels the numerator of the previous quantity until the units of the answer are obtained. (See The Factor Label Method.)

1.1-3. Determining Molar Mass Exercise

EXERCISE 1.1:

Determine the molar masses of the following. Express all answers to the nearest whole number.

N_2F_4

Atomic weight of N ____________

Atomic weight of F ____________

Molar mass of N_2F_4 ____________ g/mol

$Ca_3(PO_4)_2$

Atomic weight of Ca ____________

Atomic weight of P ____________

Atomic weight of O ____________

Molar mass of $Ca_3(PO_4)_2$ ____________ g/mol

1.1-4. Mass-Mole Conversion Exercises

EXERCISE 1.2:

What is the mass of 3.24 mol N_2O_5?

Molar mass M_m = ____________ g/mol

Mass m = ____________ g

How many moles of N_2O_5 are in 12.7 g?

Moles n = ____________ mol

1.1-5. Moles-Items Exercise

<u>EXERCISE 1.3</u>:

How many Al atoms are present in 0.065 g Al?

Moles of atoms $n =$ ______________ mol

Individual atoms $N =$ ______________ atoms

1.1-6. Ideal Gas Law

The number of moles of molecules in a gas can also be determined with the ideal gas law.

$$PV = nRT \qquad \text{Ideal Gas Law} \tag{1.1}$$

- P is the pressure of the gas in atmospheres. 1 atm = 760 torr
- V is its volume in liters.
- n is the number of moles of gas.
- $R = 0.08206$ L·atm·K^{-1}·mol^{-1} is the ideal gas law constant.
- T is the temperature on the Kelvin scale (K = °C + 273.15).

1.1-7. Gas Law Exercise

<u>EXERCISE 1.4</u>:

How many moles of H_2 are in a 3.06 L container at 22 °C if its pressure is 742 torr?

$P =$ ______________ atm

$V =$ ______________ L

$R = 0.08206$ L·atm·K^{-1}·mol^{-1}

$T =$ ______________ K

$n =$ ______________ mol H_2

1.2 Determining Chemical Formulas

Introduction

The composition of a compound is given in terms of the mass percents of its component elements. In this section, we show how these fractions can be determined from the chemical formula of the compound and how the chemical formula can be determined from the fractions.

Objectives

- Determine the mass composition of a compound from experimental data.
- Determine the mass composition from the formula of the compound.
- Determine the amount of one element that is combined with a known amount of another element or is present in a known amount of compound.
- Determine the simplest formula of a compound from the relative amounts of each of the elements present in a sample.

- Determine a molecular formula from its simplest formula and molar mass.
- Use the empirical formula and the molar mass of a substance to determine its molecular formula.

1.2-1. Experimental Mass Composition

The mass fraction of an element in a compound is the mass of the element divided by the mass of the compound in which it is found.

$$\text{mass fraction of element A} = \frac{\text{mass of element A in compound}}{\text{mass of compound}}$$

The ***mass percent*** of an element in a compound is its mass fraction expressed as a percent.

$$\text{mass percent of element A} = \text{mass fraction of element A} \times 100\%$$

The ***elemental composition*** of a compound is frequently given by the mass percents of the elements. As shown in the following example, the elemental composition of lead(II) chloride is 74.4% Pb and 25.6% Cl by mass.

EXAMPLE:

Determine the percent lead in a sample if a 1.062 g sample contains 0.791 g Pb.

$$\%\text{ mass of element} = \frac{0.791\text{ g Pb}}{1.062\text{ g compound}} \times 100\% = 74.4\%\text{ Pb}$$

1.2-2. Composition Exercise

EXERCISE 1.5:

A 0.2986 g sample of an oxide of iron contains 0.2161 g Fe. What is the percent iron in the sample?

$$\frac{\_\_\_\_\text{ g Fe}}{\_\_\_\_\text{ g compound}} \times 100\% = \_\_\_\_\ \%\text{ Fe}$$

1.2-3. Mass Composition from Chemical Formulas

The elemental composition of a compound can be determined from its formula because its molar mass and the mass contributed by each element to its molar mass are known.

EXAMPLE:

One mole of $PbCl_2$ contains:

$$\begin{aligned}(1 \text{ mol Pb})(207 \text{ g/mol Pb}) + (2 \text{ mol Cl})(35.5 \text{ g/mol Cl}) &= 207 \text{ g Pb} + 71.0 \text{ g Cl} \\ &= 278 \text{ g PbCl}_2\end{aligned}$$

Consequently, 278 g of $PbCl_2$ contains 207 g Pb and 71.0 g Cl, so the elemental composition of lead chloride can be expressed as follows:

$$\frac{207 \text{ g Pb}}{278 \text{ g of PbCl}_2} \times 100\% = 74.5\% \text{ Pb}$$

and

$$\frac{71.0 \text{ g Cl}}{278 \text{ g of PbCl}_2} \times 100\% = 25.5\% \text{ Cl}$$

In summary, one molar mass of A_aB_b contains:

- (a mol A)(molar mass of A) grams of A
- (b mol B)(molar mass of B) grams of B

Thus, its elemental composition can be determined as follows:

$$\%\text{A in } A_aB_b = \frac{a \times \text{ molar mass of A}}{\text{molar mass of } A_aB_b} \times 100\%$$

and

$$\%\text{B in } A_aB_b = \frac{b \times \text{molar mass of B}}{\text{molar mass of } A_aB_b} \times 100\%$$

1.2-4. Mass Percent Exercise

EXERCISE 1.6:

What is the mass percent of Na in Na_2SO_4? Express your answer as a percent to the nearest whole number.

The mass of one mole of Na_2SO_4 is:

______________ g

The mass of Na in one mole of Na_2SO_4 is:

______________ g

The fraction of the mass of Na_2SO_4 that is due to sodium expressed as a percent is:

______________ %

1.2-5. Mass Percent Exercise

EXERCISE 1.7:

Determine the mass percent of P in $Ca_3(PO_4)_2$. Express your answer as a percent to the nearest whole number.

The mass of one mole of $Ca_3(PO_4)_2$ is:

______________ g

The mass of P in one mole of $Ca_3(PO_4)_2$ is:

______________ g

The fraction of the mass of $Ca_3(PO_4)_2$ that is due to phosphorus expressed as a percent is:

______________ %

1.2-6. Using Mass Percents

While an elemental mass fraction has no units, units are implied in factor label problems because the fraction is determined to be (mass of element)/(mass of compound). Consequently, mass fractions can be used to convert between the mass of an element and the mass of the compound. Similarly, the mass percent of an element in a compound can be viewed as the mass of the element present in 100 g of compound. Thus, the fact that XY is 30% X by mass implies that there are 30 g X/100 g XY. Furthermore, the sum of the elemental percents of all the elements in a compound must sum to 100%, so we can deduce the percent of one element in a compound if we know the percents of all other elements in the compound. Thus, if XY is 30% X by mass, then it must also be 70% Y by mass.

EXAMPLE:

Lead chloride is 74.4% lead by mass. How much lead is present in 23.4 g of lead chloride?

The percent is expressed as 74.4 g Pb/100 g compound, which is the factor required for the conversion.

$$23.4 \text{ g compound} \times \frac{74.4 \text{ g Pb}}{100 \text{ g compound}} = 17.4 \text{ g Pb}$$

What is the percent chloride in lead chloride?

The compound contains only Pb and Cl, so the sum of the percents of the two elements must be 100%. However, $PbCl_2$ is 74.4% Pb, so

$$\%\text{Cl} = 100\% - \%\text{Pb} = 100.0 - 74.4 = 25.6\%\text{Cl}$$

Thus, $PbCl_2$ is 74.4% Pb and 25.6% Cl by mass.

1.2-7. Composition Exercise

EXERCISE 1.8:

Hexane (C_6H_{14}) is 83.7% carbon by mass.

What portion, expressed as a percent, of the mass of hexane is due to hydrogen?

%H = ____________ %

How many grams of hexane contain 13.6 g C?

$$\_\_\_\_\ \text{g C} = \frac{\_\_\_\_\ \text{g } C_6H_{14}}{\_\_\_\_\ \text{g C}} = \_\_\_\_\ \text{g } C_6H_{14}$$

1.2-8. Empirical Formula

The elemental composition can be used to determine the ratio of elemental masses in a compound. Molar masses can then be used to convert the ratio of elemental masses into one of moles, and the ratio of moles is the ratio of subscripts in the compound. We cannot determine the actual subscripts without more information, but we can determine the simplest set of integers that results in the correct ratios. The formula of a compound that uses this simplest set of integers is called the ***empirical formula*** or the ***simplest formula***. To determine the empirical or simplest formula of a compound from its elemental composition:

1 Convert the amount of each element in a sample into moles of the element.

2 Determine the ratio of the moles by dividing each by the smallest.

3 If the result of Step 2 is not an integer, convert the ratio to a ratio of simple whole numbers. This is most easily accomplished by identifying the fraction that corresponds to the decimal, and then multiplying the ratio by the integer that makes the ratio an integer. See Table 1.1: Some Common Decimals and their Multipliers.

Step 2	Multiplier
0.125	8
0.167	6
0.200	5
0.250	4
0.333	3
0.375	8

Step 2	Multiplier
0.5	2
0.625	8
0.667	3
0.75	4
0.833	6
0.875	8

Table 1.1: Some Common Decimals and their Multipliers

For example, to convert a H:C mole ratio in Step 2 of 2.667 to a ratio of small whole numbers, you can recognize that the number means 2.667 mol H/1 mol C and that 0.667, which is a ratio of 2/3 or use the above table to determine that the multiplier must be 3. Multiply the numerator and denominator of the ratio by 3 to eliminate the fraction. The result is 3(2.667)/3(1) = 8 mol H/3 mol C. The formula of the compound is C_3H_8.

1.2-9. Empirical Formula Exercise

EXERCISE 1.9:

6.84 g of an oxide of chromium is found to contain 4.68 g Cr. What is the empirical formula of the oxide? Assume that the compound contains only Cr and O. Express all answers to three significant digits.

The number of moles of each element in the sample is:

moles of Cr ($M_m = 52.0$ g/mol) in the sample: ______________ mol Cr

moles of O in the sample: ______________ mol O

The ratio of the larger number of moles to the smaller number of moles (mol O/mol Cr) is:

____

The ratio determined in the previous step as a ratio of whole numbers (For example, 1.33 mol O/mol Cr would be expressed as 4/3) is:

____

The empirical formula is the following. (Denote any subscripts with an underscore. For example, NH_3 for NH_3.)

____

1.2-10. Empirical Formula Exercise

EXERCISE 1.10:

When hydrocarbons (compounds that contain only C and H) are burned, all of the carbon is converted into CO_2 and all of the hydrogen into H_2O. What is the empirical formula of a hydrocarbon that produces 0.200 mol CO_2 and 0.125 mol H_2O when burned?

The number of moles of carbon in the sample is:

____

The number of moles of hydrogen in the sample is:

____

The ratio of the larger to the smaller number of moles is:

____

The above number expressed as a ratio of whole numbers is:

____

The empirical formula of the hydrocarbon is the following. (Denote any subscripts with an underscore. For example, NH_3 for NH_3.)

____

1.2-11. Empirical Formulas from Elemental Compositions

To determine the empirical formula of a compound from its percent composition, use the percents as if they were masses in grams and proceed as in the previous topic.

Different samples of a compound are often used to determine each element in an elemental analysis, so compositions are usually presented as mass percents rather than absolute masses. The mass of each element in any amount of sample can be determined with the mass percents, so any sample size can be used. The most convenient sample size to use with mass percents is 100 g because the masses of the elements present in a 100 g sample are equal to the mass percents. For example, 100 g of a compound that is 60% C contains 60 g C or $60/12 = 5$ mol C. To determine an empirical formula from mass percents:

1 Divide the mass percent of each element by its molar mass to determine the number of moles of the element present in 100 g of sample.

2 Divide each of the moles determined in Step 1 by the smallest number of moles to get simple ratios.

3 If any of the results of Step 2 are not integers, multiply all of the numbers by the integer that makes them integers.

4 The integers determined in Step 3 are the subscripts in the empirical formula.

1.2-12. Empirical Formula from Elemental Composition Exercise

EXERCISE 1.11:

A hydrocarbon (a compound that contains only carbon and hydrogen) is found to be 82.66% C and 17.34% H by mass. What is the empirical formula of the hydrocarbon? Use molar masses of 12.01 g/mol and 1.008 g/mol for C and H, respectively.

The number of moles of C in 100 g of compound is:

____

The number of moles of H in 100 g of compound is:

____

The ratio expressed as a decimal of the smaller number to the larger number of moles is:

____

The ratio in Step 3 expressed as a ratio of whole numbers is:

____

The empirical formula is the following. (Denote any subscripts with an underscore. For example, NH_3 for NH_3.)

____

1.2-13. Molecular Formulas

A molecular formula of a compound, which shows the actual number of atoms present in a molecule, can be determined from its empirical formula and molar mass.

An empirical formula gives the simplest whole number ratios of the atoms, while a ***molecular formula*** shows the actual number of atoms present in each molecule. A molecular formula must contain an integral number of empirical units, so the molar mass of a compound must be an integer times the molar mass of the empirical unit. Consider the following table of compounds with the empirical formula CH; i.e., they all have molecular formulas of the type $(CH)_n$, where n is an integer. The molar mass on one empirical unit (CH) is 13 g/mol, so the molar mass of $(CH)_n$ is $13n$.

molecular formula	n	molar mass (g/mol)
$C_{12}H_{12}$	12	$13 \times 12 = 156$
C_6H_6	6	$13 \times 6 = 78$
C_4H_4	4	$13 \times 4 = 52$

Table 1.2

We use the fact that molar mass of the compound = $n \times$ molar mass of the empirical unit to determine the value of n as follows:

$$n = \frac{\text{molar mass of compound}}{\text{molar mass of empirical unit}} \qquad \text{empirical units} \tag{1.2}$$

Once we have the value of n, we can write the molecular formula by simply multiplying each of the subscripts in the empirical formula by n. For example, to determine the molecular formula of a compound with an empirical formula of CH_2 (M_m = 14 g/mol) and a molar mass of 112 g/mol, we would first determine n as

$$n = \frac{112 \text{ g/mol}}{14 \text{ g/mol}} = 8$$

The compound contains eight empirical units: $(CH_2)_8$, which would be written as C_8H_{16}.

1.2-14. Molecular Formula Exercise

EXERCISE 1.12:

Write the empirical formula for each of the following molecular formulas. (Denote any subscripts with an underscore. For example, NH_3 for NH_3.)

$C_4H_{10}N_4$: ________ $C_{12}H_{24}N_5$: ________ $C_8H_8N_4$: ________

1.2-15. Molecular Formula from Empirical Formula Exercise

EXERCISE 1.13:

What is the molecular formula of a compound that has an empirical formula of C_2H_4O and a molar mass of 88 g/mol?

$$n = \frac{\_\_\_\_\_\_ \text{ g/mol}}{\_\_\_\_\_\_ \text{ g/mol}} = \_\_\_\_\_\_$$

The empirical formula of the compound is the following. (Denote any subscripts with an underscore. For example, NH_3 for NH_3.)

____

1.2-16. Molecular Formula Exercise

EXERCISE 1.14:

What is the molecular formula of a compound that is 64.27% C, 7.19% H, and 28.53% O and has a molar mass of about 220 g/mol?

100.00 g of this compound contains how many moles of each element?

C ______________ mol H ______________ mol O ______________ mol

The number of moles of each element divided by the smallest number of moles is:

C ______________ mol H ______________ mol O ______________ mol

The empirical formula of the compound is the following. (Denote any subscripts with an underscore. For example, NH_3 for NH_3.)

____

The number of empirical units present in one molecular unit is:

____

The molecular formula is the following. (Denote any subscripts with an underscore. For example, NH_3 for NH_3.)

____

1.2-17. Molecular Formula from Combustion Exercise

EXERCISE 1.15:

It is common to determine formulas of organic compounds by burning them and determining the mass fractions of carbon and hydrogen from the amounts of CO_2 and H_2O that are produced in the combustion. If the compound contains oxygen, the mass of oxygen must be determined from the total mass of the sample and the masses of C and H that it contains.

What is the empirical formula of ascorbic acid (vitamin C) if combustion of 0.579 g of ascorbic acid produces 0.868 g of CO_2 and 0.237 g H_2O? Ascorbic acid also contains oxygen.

Convert mass of CO_2 and H_2O to moles.

moles of CO_2 produced: ______________ mol CO_2

moles of C present in the CO_2: ______________ mol C

moles of H_2O produced: ______________ mol H_2O

moles of H present in the H_2O: ______________ mol H

The sample contains oxygen, so its mass must be determined by difference. Therefore, the mass of C and H must be determined from the number of moles above. Note: this step would not be necessary if the sample contained no oxygen. We would simply determine the mol H/mol C ratio with the numbers of moles determined above to get the empirical formula.

mass of C in sample: ______________ g C

mass of H in sample: ______________ g H

mass of oxygen in sample: ______________ g O

moles of oxygen in sample: ______________ mol O

Determine the mole ratios.

mol C/mol C = ______________

mol H/mol C = ______________

mol O/mol C = ______________

Multiplier to be used to convert all of the above to integers:

____

The subscripts in the empirical formula:

subscript of C = ______________

subscript of H = ______________

subscript of O = ______________

The molar mass of ascorbic acid is 176 g/mol. What is its molecular formula?

The molar mass of the empirical unit = ______________ g/mol

The number of empirical units in a molecular unit = ______________ units

The subscripts in the molecular formula:

subscript of C = ______________

subscript of H = ______________

subscript of O = ______________

1.3 Substance or Composition Stoichiometry

Introduction

In a composition stoichiometry problem, the amount of one substance that is combined with another is determined with the use of the ratios of the subscripts in the chemical formula.

Objectives

- Determine and use stoichiometric links derived from chemical formulas.

1.3-1. Stoichiometric Link Video

A video or simulation is available online.

1.3-2. Stoichiometric Links and Chemical Formulas

The stoichiometric links for a substance are formed from the subscripts in a chemical formula.

A ***stoichiometric link*** is the ratio of the number of moles of one substance to the number of moles of another substance with which it combines. The stoichiometric link between two elements in a compound equals the ratio of the subscripts of the two elements in the compound. Consider the example of ammonia shown in Figure 1.1. One molecule of NH_3 contains one nitrogen atom and three hydrogen atoms, so we can write the following stoichiometric links between NH_3, N, and H.

$\frac{1 \text{ mol N}}{3 \text{ mol H}}$	$\frac{1 \text{ mol N}}{1 \text{ mol NH}_3}$	$\frac{3 \text{ mol H}}{1 \text{ mol NH}_3}$

Table 1.3

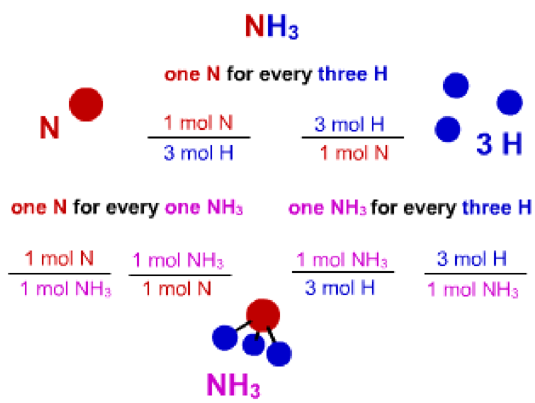

Figure 1.1: Substance Stoichiometry in NH_3

The stoichiometric links available from the formula H_2SO_4 are:

Conversion factors using H in $\mathbf{H}_2SO_4$			Conversion factors using S in $H_2\mathbf{S}O_4$			Conversion factors using O in $H_2S\mathbf{O}_4$		
$\frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{SO}_4}$	$\frac{2 \text{ mol H}}{1 \text{ mol S}}$	$\frac{2 \text{ mol H}}{4 \text{ mol O}}$	$\frac{1 \text{ mol S}}{1 \text{ mol H}_2\text{SO}_4}$	$\frac{1 \text{ mol S}}{2 \text{ mol H}}$	$\frac{1 \text{ mol S}}{4 \text{ mol O}}$	$\frac{4 \text{ mol O}}{1 \text{ mol H}_2\text{SO}_4}$	$\frac{4 \text{ mol O}}{2 \text{ mol H}}$	$\frac{4 \text{ mol O}}{1 \text{ mol S}}$

Table 1.4

1.3-3. Using the Stoichiometric Link

Stoichiometric links can be combined with the factor label method to determine the amount of any element in a compound that is combined with a known amount of any other element in the compound.

The units of the denominator of the stoichiometric link must be the same as the given quantity, and the units of the numerator must be the same as those of the desired quantity. Thus, to **convert the amount of one atom or ion into the amount of another in the same compound, multiply the number of moles of a given substance by the appropriate stoichiometric link derived from the subscripts in the chemical formula**.

$$\text{moles of given} \times \frac{\text{subscript of desired}}{\text{subscript of given}} = \text{moles of desired} \tag{1.3}$$

1.3-4. Mass-Mass Conversion

We have seen that the heart of a substance stoichiometry problem is multiplying the given number of moles by the appropriate stoichiometric link to obtain the number of moles of the desired substance. We now combine that operation with the molar masses of the given and desired substances to determine the mass of one substance (the desired substance) that is combined with a given mass of another (the given substance). The process involves the following three conversions:

1 **mass A → mol A**: Convert the given mass into given moles with the molar mass of the given substance.

2 **mol A → mol B**: Multiply the given moles calculated in Step 1 by the appropriate stoichiometric link to obtain the desired moles.

3 **mol B → mass B**: Convert the desired moles determined in Step 2 into grams with the molar mass of the desired substance.

Of course, all three steps can be combined into one extended multiplication with the factor label method. For example, the following shows how to determine the number of grams of oxygen ($M_m = 16.0$ g/mol) that are combined with 12.2 g of aluminum ($M_m = 27.0$ g/mol) in Al_2O_3.

$$12.2\ \cancel{\text{g Al}} \times \frac{1\ \cancel{\text{mol Al}}}{27.0\ \cancel{\text{g Al}}} \times \frac{3\ \cancel{\text{mol O}}}{2\ \cancel{\text{mol Al}}} \times \frac{16.0\text{ g O}}{1\ \cancel{\text{mol O}}} = 10.8\text{ g O}$$

We first divide the given mass of Al by its molar mass to obtain moles of Al. The moles of Al are then multiplied by the ratio of subscripts (stoichiometric link) to obtain the moles of O. Finally, the moles of O are multiplied by the molar mass of O to obtain grams of O. Note that all of the units cancel except grams of O, the desired quantity.

1.3-5. Mole Atom-Mole Molecule Conversion Exercise

EXERCISE 1.16:

How many moles of $MgCl_2$ contain 0.64 mol Cl atoms?

$$\_\_\_\_\ \text{mol Cl} \times \frac{\_\_\_\_\ \text{mol MgCl}_2}{\_\_\_\_\ \text{mol Cl}} = \_\_\_\_\ \text{mol MgCl}_2$$

1.3-6. Mole Atom-Mole Atom Conversion Exercise

EXERCISE 1.17:

How many moles of hydrogen atoms are in a sample of C_6H_{14} that contains 0.25 mol C?

$$\_\_\_\_\ \text{mol C} \times \frac{\_\_\_\_\ \text{mol H}}{\_\_\_\_\ \text{mol C}} = \_\_\_\_\ \text{mol H}$$

1.3-7. Mass Atom-Mass Molecule Conversion Exercise

EXERCISE 1.18:

What mass of Fe_3O_4 ($M_m = 232$ g/mol) contains 12 g of iron ($M_m = 55.9$ g/mol)?

$$\boxed{}\ \text{g Fe} \times \frac{\boxed{}\ \text{mol Fe}}{\boxed{}\ \text{g Fe}} \times \frac{\boxed{}\ \text{mol Fe}_3\text{O}_4}{\boxed{}\ \text{mol Fe}} \times \frac{\boxed{}\ \text{g Fe}_3\text{O}_4}{\boxed{}\ \text{mol Fe}_3\text{O}_4} = \boxed{}\ \text{g Fe}_3\text{O}_4$$

1.3-8. Mass Atom-Mass Atom Conversion Exercise

EXERCISE 1.19:

What mass of Fe ($M_m = 55.9$ g/mol) is combined with 26.3 g chlorine ($M_m = 35.5$ g/mol) in $FeCl_3$?

$$\boxed{}\ \text{g C} \times \frac{\boxed{}\ \text{mol Cl}}{\boxed{}\ \text{g Cl}} \times \frac{\boxed{}\ \text{mol Fe}}{\boxed{}\ \text{mol Cl}} \times \frac{\boxed{}\ \text{g Fe}}{\boxed{}\ \text{mol Fe}} = \boxed{}\ \text{g Fe}$$

1.4 Balancing Chemical Equations

Introduction

Neither the identity nor the number of atoms is changed in a chemical reaction, so chemical equations are balanced to assure that the number of each type of atom is the same on both sides. This is done by changing the number of each reacting and produced molecule by placing coefficients in front of each species. In this section, we show how to balance simple chemical equations by inspection.

Objectives

- Balance a chemical equation by inspection.

1.4-1. Balancing Chemical Equations Video

A video or simulation is available online.

1.4-2. Procedure for Balancing Equations

Chemical equations are balanced to assure that the number of each type of atom is the same on both sides of the equation. Only coefficients (not subscripts) can be changed to balance a chemical equation.

The following steps should lead to a balanced equation:

1 Pick the molecule with the greatest number of atoms and set its coefficient to "1" unless another choice is obviously better. For example, sometimes a "2" must be used to assure an even number of one of the atoms.

2 Determine which atoms are fixed by the coefficient set in Step 1, then balance those atoms on the other side of the equation.

3 Determine which atoms are fixed by the coefficient(s) created in Step 2, then balance those atoms on the other side of the equation.

4 Repeat Step 3 until the equation is balanced.

Note that coefficients of "1" are not usually included in the balanced equation.

EXAMPLE:

As an example, we will follow the steps above to balance the following chemical equation:

$$\_\_\_\_\_\_ \text{HCl} + \_\_\_\_\_\_ \text{MnO}_2 \rightarrow \_\_\_\_\_\_ \text{MnCl}_2 + \_\_\_\_\_\_ \text{H}_2\text{O} + \_\_\_\_\_\_ \text{Cl}_2$$

1 Make the coefficient of either MnO_2 or $MnCl_2$ one. We choose MnO_2.

$$\_\_\_\_\_\_ \text{HCl} + \mathbf{1}\ \text{MnO}_2 \rightarrow \_\_\_\_\_\_ \text{MnCl}_2 + \_\_\_\_\_\_ \text{H}_2\text{O} + \_\_\_\_\_\_ \text{Cl}_2$$

2 The coefficient used in Step 1 fixes the number of Mn atoms at 1 and O atoms at 2, so we balance the Mn atoms with a coefficient of 1 for $MnCl_2$ and the oxygen atoms with a coefficient of 2 for water.

$$\_\_\_\_\_\_ \text{HCl} + 1\ \text{MnO}_2 \rightarrow \mathbf{1}\ \text{MnCl}_2 + \mathbf{2}\ \text{H}_2\text{O} + \_\_\_\_\_\_ \text{Cl}_2$$

3 The coefficient of water fixes the number of hydrogen atoms at four, so we balance the H atoms with a coefficient of 4 for HCl. Note that the coefficient of $MnCl_2$ does not fix the number of Cl atoms because it is not the only source of Cl.

$$\mathbf{4}\ \text{HCl} + 1\ \text{MnO}_2 \rightarrow 1\ \text{MnCl}_2 + 2\ \text{H}_2\text{O} + \_\_\_\_\_\_ \text{Cl}_2$$

4 The coefficient of HCl fixes the number of chlorine atoms at four, but there are already 2 Cl atoms in 1 $MnCl_2$, so we balance the Cl atoms on the other side of the equation with a coefficient of 1 for Cl_2.

$$4\ \text{HCl} + 1\ \text{MnO}_2 \rightarrow 1\ \text{MnCl}_2 + 2\ \text{H}_2\text{O} + \mathbf{1}\ \text{Cl}_2$$

5 Each side of the equation contains 4 H atoms, 1 Mn atom, 2 O atoms, and 4 Cl atoms. The equation is now balanced, but ones are not usually written. Thus, the balanced equation is usually written as shown in the last step.

$$4\ \text{HCl} + \text{MnO}_2 \rightarrow \text{MnCl}_2 + 2\ \text{H}_2\text{O} + \text{Cl}_2$$

1.4-3. Balancing Equations Exercise

EXERCISE 1.20:

Balance the following equations with the smallest whole-number coefficients. Include coefficients of "1" in your answer.

$$\_\_\_\_\_\_ \text{N}_2 + \_\_\_\_\_\_ \text{O}_2 \rightarrow \_\_\_\_\_\_ \text{N}_2\text{O}_5$$

$$\_\_\_\_\_\_ \text{Na} + \_\_\_\_\_\_ \text{H}_2\text{O} \rightarrow \_\_\_\_\_\_ \text{NaOH} + \_\_\_\_\_\_ \text{H}_2$$

$$\_\_\_\_\_\_ \text{P}_4 + \_\_\_\_\_\_ \text{Cl}_2 \rightarrow \_\_\_\_\_\_ \text{PCl}_3$$

$$\_\_\_\_\_\_ \text{C}_6\text{H}_{12}\text{O}_6 + \_\_\_\_\_\_ \text{O}_2 \rightarrow \_\_\_\_\_\_ \text{CO}_2 + \_\_\_\_\_\_ \text{H}_2\text{O}$$

1.5 Reaction Stoichiometry

Introduction

The ratios of the coefficients of a balanced equation are conversion factors that allow us to calculate the amount of one substance that is produced by or reacts with a given amount of another substance. The only difference between this process and the one used to determine how much of one element was combined with a given amount of another element in a compound is the stoichiometric ratio or link: in one, the stoichiometric link is the ratio of the subscripts in the chemical formula; in the other, it is the ratio of the coefficients in the balanced equation. All other operations are the same in the two problem types.

Objectives

- Write the stoichiometric ratio relating two substances involved in a chemical reaction.
- Use the ratio to convert the amount of one substance involved in the reaction to the chemically equivalent amount of another substance in the same reaction.
- Identify the limiting reactant in a reaction.
- Determine the amount of product formed or of reactant consumed from the amount of limiting reactant that reacts.
- Determine the percent yield given the actual yield of a reaction or use the percent yield to determine the actual yield.
- Determine the complete composition of a reaction mixture after the reaction is complete.

1.5-1. Stoichiometric Links in Chemical Reactions

Stoichiometric links formed from the coefficients of balanced chemical equations are used to convert between equivalent amounts of reactants and products in a reaction.

Consider the following balanced chemical equation:

$$N_2 + 3\ H_2 \rightarrow 2\ NH_3$$

The coefficients indicate the relative number number of molecules that react, not the absolute number. That is, the equation does not indicate that three moles of H_2 react. Rather, it indicates that 3 mol H_2 react for every 1 mol N_2 that reacts or for every 2 mol NH_3 that form. Thus, we can write the following stoichiometric links for the reaction.

$\frac{1\text{ mol } N_2}{2\text{ mol } NH_3}$	$\frac{1\text{ mol } N_2}{3\text{ mol } H_2}$	$\frac{2\text{ mol } NH_3}{3\text{ mol } H_2}$

Table 1.5

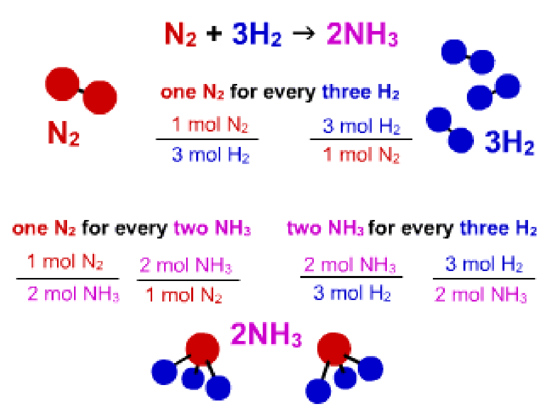

Figure 1.2: Reaction Stoichiometry in the Formation of NH_3 Reaction

1.5-2. Using Stoichiometric Links for Chemical Reactions

The stoichiometric links produced by the coefficients in a balanced equation can be used to determine the number of moles of one substance that are produced by or react with a given number of moles of another substance in the equation.

EXAMPLE:

The following shows how to determine the number of moles of nitrogen that are required and how many moles of NH_3 are produced in the reaction of 3.6 moles of hydrogen in the following:

$$3\ H_2 + N_2 \rightarrow 2\ NH_3$$

$$3.6 \text{ mol } H_2 \times \frac{1 \text{mol } N_2}{3 \text{ mol } H_2} = 1.2 \text{ mol } N_2 \text{ are required}$$

$$3.6 \text{ mol } H_2 \times \frac{2 \text{ mol } NH_3}{3 \text{ mol } H_2} = 2.4 \text{ mol } NH_3 \text{ are produced}$$

Note that the stoichiometric link is simply the ratio of the coefficients in the balanced chemical equation. As in all applications of the factor label method, the units of the denominator of the stoichiometric link must be the same as the given quantity and the units of the numerator are those of the result.

1.5-3. Mole-Mole Conversion Exercise

EXERCISE 1.21:

How many moles of hydrogen are required to produce 2.8 mol NH_3? The chemical equation is

$$N_2 + 3\ H_2 \rightarrow 2\ NH_3$$

$$\_\_\_\_ \text{ mol } NH_3 \times \frac{\_\_\_\_ \text{ mol } H_2}{\_\_\_\_ NH_3} = \_\_\_\_ \text{ mol } H_2$$

1.5-4. Method for Mass-Mass Conversions

We finish this lesson by showing how to determine the mass of one substance that reacts with or is produced by the reaction of a given mass of another substance in the chemical equation. The process, which is identical to that used in determining the mass of one element that is combined with a given mass of another element in a compound, involves the following three conversions:

1. **mass A → mol A**: Use the molar mass of the given compound to convert its mass to moles.
2. **mol A → mol B**: Use the stoichiometric link (ratio of coefficients) to convert the number of moles of given compound determined in Step 1 into the equivalent number of moles of desired substance.
3. **mol B → mass B**: Use the molar mass of the desired substance to convert the number of moles determined in Step 2 into the mass of the desired substance.

The three steps can be combined into one factor-label setup as shown in the following Example.

EXAMPLE:

The mass of Na_2O (M_m = 62 g/mol) that is produced in the reaction of 6.0 g Na (M_m = 23 g/mol) by the reaction $4\ Na + O_2 \rightarrow 2\ Na_2O$ is determined as follows:

$$6.0\text{ g Na} \times \frac{1\text{ mol Na}}{23\text{ g Na}} \times \frac{2\text{ mol Na}_2\text{O}}{4\text{ mol Na}} \times \frac{62\text{ g Na}_2\text{O}}{1\text{ mol Na}_2\text{O}} = 8.1\text{ g Na}_2\text{O}$$

$$6.0\text{ g Na} \rightarrow 0.26\text{ mol Na} \rightarrow 0.13\text{mol Na}_2\text{O} \rightarrow 8.1\text{ g Na}_2\text{O}$$

1.5-5. Mass-Mass Conversion Exercise

EXERCISE 1.22:

How many grams of fluorine must react to produce 24 g PF_5 (M_m = 126 g/mol)?

F_2 (M_m = 38 g/mol) reacts with P_4 (M_m = 126 g/mol) by the following reaction:

$$P_4 + 10\ F_2 \rightarrow 4\ PF_5$$

$$\boxed{}\text{ g PF}_5 \times \frac{\boxed{}\text{ mol PF}_5}{\boxed{}\text{ g PF}_5} \times \frac{\boxed{}\text{ mol F}_2}{\boxed{}\text{ mol PF}_5} \times \frac{\boxed{}\text{ g F}_2}{\boxed{}\text{ mol F}_2} = \boxed{}\text{ g F}_2$$

1.5-6. Limiting Reactants

Thus far, we have determined the amount of substance that reacts with or is formed by the reaction of another substance. However, there is usually more than one reactant and the reactants are not usually added in stoichiometric ratios. In such cases, one of the reactants, known as the ***limiting reactant***, is consumed before any other reactant. The other reactants are said to be in excess because they are still available after the limiting reactant is consumed.

The limiting reactant is identified as the reactant that is capable of producing the least amount of product. Thus, one way to determine which of several reactants is the limiting reactant is to determine the amount of product each reactant is capable of producing. The limiting reactant is the one that is capable of producing the least. Note, that the limiting reactant is not necessarily the reactant present in the smallest mass nor in the smallest number of moles.

To determine the limiting reactant, you would determine the number of moles of a substance B that is produced or reacts with a given number of moles of reactant A. The moles of B is formed from reactant A:

$$\text{mol A} \times \frac{\text{coefficient B}}{\text{coefficient A}} = \text{ mol B}$$

However, this can be rewritten as follows:

$$\frac{\text{mol A}}{\text{coefficient A}} \times \text{ coefficient B} = \text{ mol B}$$

The coefficient of B is constant, so the smallest amount of B would be produced by the reactant with the smallest mol/coefficient ratio. We conclude that **the limiting reactant is that reactant with the smallest (mol A/coefficient A) ratio**.

The amount of any product that forms or reactant that reacts is equal to the (reactant moles)/(reactant coefficient) ratio of the limiting reactant times the coefficient of the product or reactant whose amount is to be determined.

1.5-7. Mole-Mole Limiting Reactant Exercise

EXERCISE 1.23:

How many moles of NF_3 can be produced from the reaction of 0.50 mol N_2 and 0.90 mol F_2 in the following reaction?

$$N_2 + 3\ F_2 \rightarrow 2\ NF_3$$

Determine mole/coefficient ratios.

N_2 ______________ F_2 ______________

The limiting reactant is

N_2
F_2

Moles of NF_3 that can be produced by the limiting reactant is

______________ mol NF_3

1.5-8. Mass-Mass Limiting Reactant Exercise

EXERCISE 1.24:

How many grams of Ag_3PO_4 (M_m = 418.6 g/mol) form in the reaction of 3.21 g $AgNO_3$ (M_m = 169.9 g/mol) and 1.65 g K_3PO_4 (M_m = 212.3 g/mol)? How much of the excess reactant remains?

$$3\ AgNO_3 + K_3PO_4 \rightarrow Ag_3PO_4 + 3\ KNO_3$$

Determine the number of moles of each reactant.

$AgNO_3$ ______________ mol K_3PO_4 ______________ mol

Determine the mol/coefficient ratios.

$AgNO_3$ ______________ K_3PO_4 ______________

Identify the limiting reactant.

$AgNO_3$
K_3PO_4

Determine the amount of product formed.

______________ g Ag_3PO_4

Determine the amount of excess reactant that is unreacted.

Mass of excess reactant that reacts: ______________ g

Mass of excess reactant that remains: ______________ g

1.5-9. Percent Yield

The mass of a product determined from the amount of limiting reactant and the stoichiometry of the reaction is known as the ***theoretical yield***. However, the theoretical yield is not usually isolated in an actual experiment. The actual yield, which is the amount that is actually isolated in the experiment, can be less than the theoretical yield for the following reasons:

- The reaction may not be extensive, so all of the limiting reactant does not react.
- Product can be lost during purification. For example, some solid may remain on the filter paper or dissolve when washed.
- Competing reactions can consume some of the reactants.

The fraction of the theoretical yield that is actually isolated expressed as a percent is called the ***percent yield***.

$$\text{percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% \qquad \text{Percent Yield} \tag{1.4}$$

<u>EXAMPLE</u>:

If stoichiometry predicts that 8.0 g of product should form, but only 6.0 g are actually obtained, the reaction would be reported to have a 75% yield.

$$\text{percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% = \frac{6.0\text{ g}}{8.0\text{ g}} \times 100\% = 75\%$$

1.5-10. Percent Yield Exercise

<u>EXERCISE 1.25</u>:

Aspirin ($C_9H_8O_4$, M_m = 180.16 g/mol) is prepared from the reaction of salicylic acid ($C_7H_6O_3$, M_m = 138.12 g/mol) and acetic anhydride ($C_4H_6O_3$, M_m = 102.09 g/mol) by the following reaction:

$$C_7H_6O_3 + C_4H_6O_3 \rightarrow C_9H_8O_4 + C_2H_4O_2$$

What is the percent yield of aspirin if the reaction of 20.00 g of salicylic acid and 17.00 g of acetic anhydride produces 22.36 g of aspirin?

theoretical yield of aspirin if salicylic acid is the limiting reactant: ________ g $C_9H_8O_4$

theoretical yield of aspirin if acetic anhydride is the limiting reactant: ________ g $C_9H_8O_4$

theoretical yield of aspirin: ________ g $C_9H_8O_4$

actual yield of aspirin: ________ g $C_9H_8O_4$

percent yield: ________ %

1.5-11. Reaction Table Lecture

A video or simulation is available online.

1.5-12. Lines of a Reaction Table

Reaction tables have three rows (initial, Δ, and final) and a column for each reactant and product in the chemical equation.

Reaction tables are completed for chemical reactions to show the amounts of all substances that react and are produced in order to determine the amounts that are present at the end of the reaction. They are constructed with three lines under the balanced equation: initial, Δ, and final.

1 **initial**: The initial line consists of the number of moles of each ingredient present before the reaction begins. Only the reactants are mixed in most reactions, so the entries under the products are zero in most reaction tables.

2 Δ: The delta (change) line shows how many moles of each reactant disappears and how many moles of each product are produced. All calculations on this line are based on the assumption that all of the limiting reactant disappears. The entries of all products are positive because they form during the reaction, but those of all reactants are negative because they disappear during the reaction.

3 **final**: The final line is the sum of the initial and delta lines and represents the final composition of the reaction mixture.

1.5-13. Reaction Table from Mass Exercise

EXERCISE 1.26:

Reaction tables are completed with either moles or concentrations, not with masses. However, initial amounts are often given as masses. In these cases, convert the masses into moles and proceed as in the previous example.

Construct the reaction table to determine the final **masses** of all substances remaining in the complete reaction of 10.00 g each of NH_3 and O_2. **Report the final masses to the nearest 0.01 g.**

	$4\ NH_3$	+	$5\ O_2$	→	4 NO	+	$6\ H_2O$	
initial		+		→		+		mol
Δ								mol
final								mol
mass								g

1.6 Exercises and Solutions

Links to view either the end-of-chapter exercises or the solutions to the odd exercises are available in the HTML version of the chapter.