General chemistry

Chapter 3

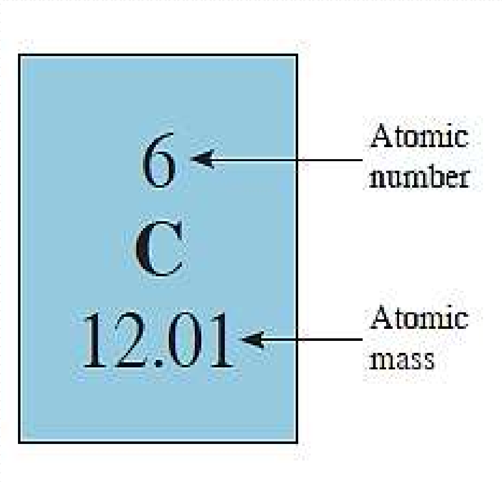
Stoichiometry

Definition of Stoichiometry

- Studying the quantitative relationships of atoms and molecules. These relationships in turn will help us to explain the composition of compounds and the ways in which composition changes.

Atomic weight

- The atomic weight or atomic mass is the weight of one atom of the element, and is expressed in the unit u= amu = atomic mass unit = Dalton (Da)
- Atomic weights of the elements is written in the periodic table in the subscript.
- ***<u>Numerically,</u>*** Atomic weight ≈ Mass number.



Molecular weight

- The **molecular weight** (called molecular mass) is the sum of the atomic weights (in amu) in the molecule.
- It is calculated weight.
- For example,

Molecular mass of H_2O = 2*(atomic mass of H) + atomic mass of O

= 2*(1.008 amu) + 16.00 amu = 18.02 amu

Molecular mass of H_2 = 2*(atomic mass of H)

= 2*(1.008 amu)

= 2 amu

Mole

- In any real situation, we deal with macroscopic samples containing enormous numbers of atoms. Therefore, it is convenient to have a special unit to describe a very large number of atoms. This special unit is the mole.
- The **mole (mol)** is the amount of a substance that contains **Avogadro's number** (N_A) of particles.

$$N_{\mathrm{A}} = 6.0221415 \times 10^{23}$$

Mole

- 1 mole of hydrogen atoms contains 6.022×10^{23} H atoms.
- 1 mole of hydrogen molecules contains 6.022×10^{23} H molecules.
- 1 mole of water molecules contains 6.022×10^{23} water molecules.
- As the mole of substances have the same number of particles, they differ in their molar mass.

Molar mass

- It is the mass (in grams or kilograms) of 1 mole of units (such as atoms or molecules) of a substance.
- ***Notes:***

A- For an element (found as atoms): the molar mass (in grams) is ***numerically*** equal to its atomic weight in amu.

- **Examples:**

1. The atomic mass of sodium (Na) is 22.99 amu and its molar mass is 22.99 g
2. The atomic mass of phosphorus is 30.97 amu and its molar mass is 30.97 g; and so on.

Molar mass

- ***Notes:***

  B- For an element (found as a molecule) or for a compound: The molar mass (in grams) is ***numerically*** equal to its molecular weight in amu.

- **Examples:**

Molecular mass of H_2O = 2*(atomic mass of H) + atomic mass of O

= 2*(1.008 amu) + 16.00 amu = 18.02 amu

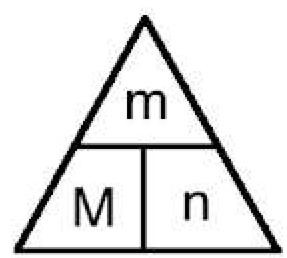
Similarly,

Molar mass of H_2O =2*(molar mass of H atoms)+ molar mass of O atoms

= 2*(1.008 g) + 16.00 g = 18.02 g

Relationship between mass and no. of moles of a substance

- A knowledge of the molar mass enables us to calculate the numbers of moles or the mass of a given quantity of a substance.
- Mass of substance (m) =No. of moles (n) X Molar mass (M)
- No. of moles= mass of substance/ Molar mass



m= mass

n= # of moles

M= molar mass

Examples

- **Zinc (Zn) is a silvery metal. How many moles of Zn are there in 23.3 g of Zn?**

From periodic table, Molar mass (M)= 65.39 g

No. of moles (n) = mass of substance (m)/Molar mass (M)

(n) = 23.3 / 65.39 =0.356 mol

- **Calculate the number of grams of lead (Pb) in 12.4 moles of lead?**

Mass of substance (m) =No. of moles (n) X Molar mass (M)

(m) = 12.4 X 207 = 2567 g

Examples

- **How many moles of CH_4 are present in 6.07 g of CH_4?**

Molar Mass of CH_4= 1*12 + 4*1= 16 g

No. of moles (n) = mass of substance (m)/Molar mass (M)

n= 6.07/16= 0.378 mol

- **Calculate the mass of chloroform ($CHCl_3$) in 1.66 moles of Chloroform?**

Molar Mass of $CHCl_3$ = 1*12 +1*1+ 3*35 = 118 g

Mass of substance (m) =No. of moles (n) X Molar mass (M)

= 1.66 * 118 = 196 g

Elemental analysis
and
Percent composition of compounds

A- Determination of Percent composition from molecular formula

- In case that the molecular formula of the compound is known, the percent composition is used to verify the purity of a compound for use in a laboratory experiment.
- This is done by comparing the result of the percent composition obtained experimentally for a sample (elemental analysis), with the percent composition calculated from the formula of the sample.

Percent composition

- The **percent composition** is the percent by mass of each element in a compound.
- If the molecular formula is known, percent composition can be calculated from the following equation:

$$\text{percent composition of an element} = \frac{\text{Mass of element in one mole of the compound}}{\text{molar mass of compound}} \times 100\%$$

- As m=n * M, and n represent the no. of moles of the element in one mole of the compound so:

$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\%$$

Problem

Phosphoric acid (H_3PO_4).Calculate the percent composition by mass of H, P, and O in this compound?

molar mass of H_3PO_4 is 97.99 g (calculated).

1 mole of H_3PO_4 contains 3 mole of H, 1 mole of P, 4 mole of O

$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\%$$

The percent by mass of each of the elements in H_3PO_4 is calculated as follows:

$$\%H = \frac{3(1.008\text{ g})\text{ H}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = 3.086\%$$

$$\%P = \frac{30.97\text{ g P}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = 31.61\%$$

$$\%O = \frac{4(16.00\text{ g})\text{ O}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = 65.31\%$$

Note: The sum of the percentages is 100.01%.

B- Determination of Percent composition from elemental analysis (experimentally)

- Elemental analysis of a compound analyze a certain mass of a sample and give the masses of individual elements in that sample mass (experimentally). So the percentage composition can be calculated as follows:
- **Percent composition of an element=**

  mass of an element/mass of the sample X 100%

Problem

- Elemental analysis of 2.5 g sample of nicotine shows that it contains 1.85 g of C, 0.218 g of H and 0.432 g of N. Calculate the percentage composition of nicotine?

- **Percent composition of an element=**

mass of an element/mass of the sample X 100%

%C = 1.85/2.5 * 100%= 74%

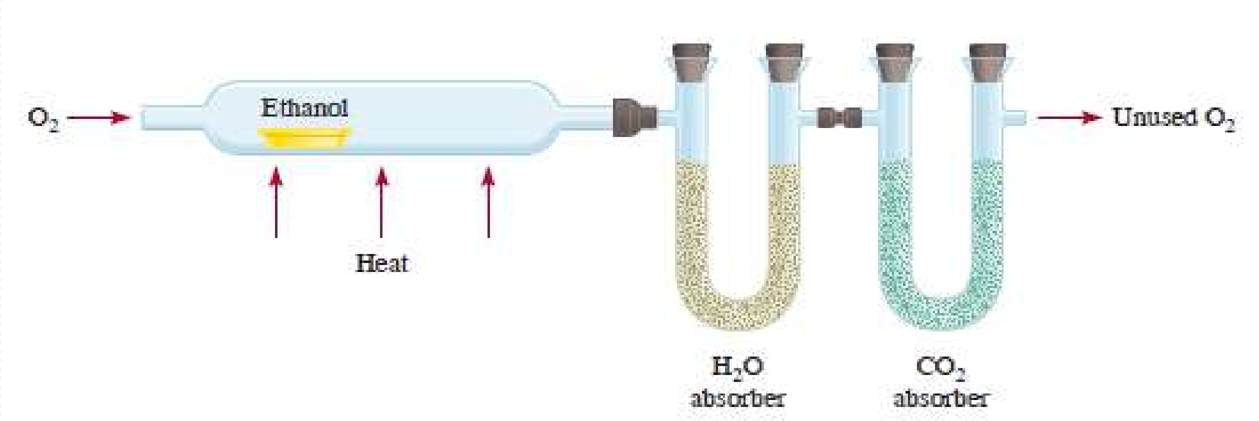
% H= 0.218/2.5*100%= 8.72%

% N= 0.432/2.5*100%= 17.3%

How elemental analysis is done Experimentally?

- Elemental analysis, determines the amounts of Carbon (C), Hydrogen (H), Nitrogen (N), Sulfur (S) and Oxygen (O) present in a sample.
- The most common technique of CHNSO elemental analysis is based on the combustion of the sample.
- The combustion products CO_2, H_2O, N_2, SO_2 are measured and thus the ratio of the elements in the original sample is determined.
- The final amounts of each element are typically given as a percentage of the original sample weight.

How elemental analysis is done Experimentally?



- When ethanol is burned, carbon dioxide (CO_2) and water (H_2O) are given off.
- 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,

- **Suppose that in one experiment the combustion of 11.5 g of a compound (contain C, H and O) produced 22.0 g of CO_2 and 13.5 g of H_2O. Calculate the mass percentage of C,H and O in the sample?**

$$1 \text{ mole of } CO_2 \triangleq 1 \text{ mole of C}$$
$$22/44 \text{ mol} \triangleq ??$$

- $n_C = 0.5$ mol So, $m_C = 0.5 \times 12 = 6$ g

$$1 \text{ mole of } H_2O \triangleq 2 \text{ mole of H}$$
$$13.5/18 \text{ mol} \triangleq ??$$

- $n_H = 1.5$ mol So, $m_H = 1.5 \times 1 = 1.5$ g

- Then,

$$\begin{aligned}\text{mass of O} &= \text{mass of sample} - (\text{mass of C} + \text{mass of H})\\ &= 11.5\text{ g} - (6.00\text{ g} + 1.51\text{ g})\\ &= 4.0\text{ g}\end{aligned}$$

- To calculate % by mass

%C = 6/11.5 * 100%= 52.17%

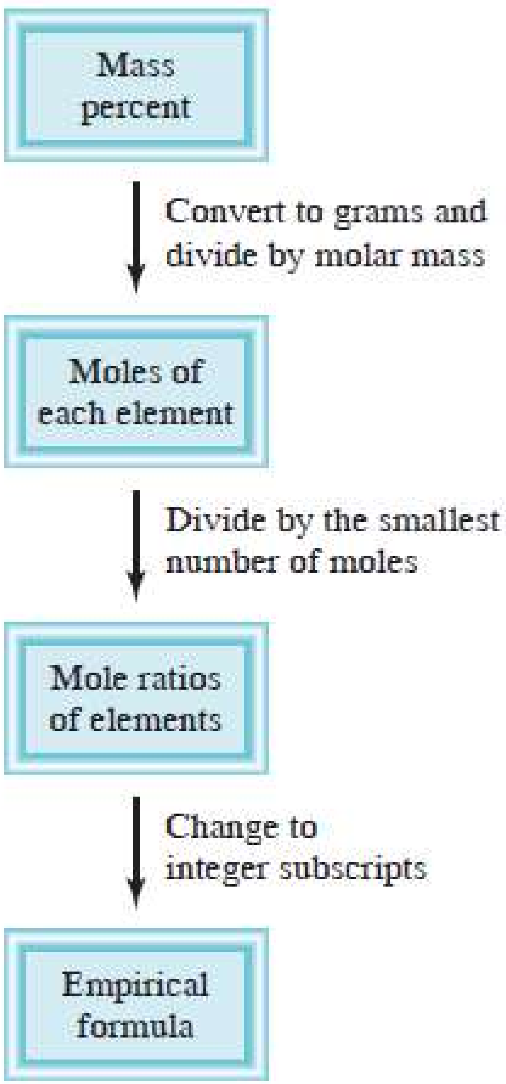
% H= 1.5/11.5*100%= 13.04%

% O= 4/11.5*100%= 34.78%

Derivation the empirical formula of the compounds from elemental analysis

Steps

Given the percent composition by mass of a compound, we can determine its empirical formula.



Problem 1

- **Ascorbic acid (vitamin C) cures scurvy. It is composed of 40.92 %(C), 4.58% (H), and 54.50% (O) by mass. Determine its empirical formula?**

1. If we have 100 g of ascorbic acid, then each percentage can be converted directly to grams. In this sample, there will be 40.92 g of C, 4.58 g of H, and 54.50 g of O.
2. we need to convert the grams of each element to moles:

$$n = m/M$$

$$n_C = 40.92/12.01 = 3.407 \text{ mol C}$$

$$n_H = 4.58/1.008 = 4.54 \text{ mol H}$$

$$n_O = 54.50/16.00 = 3.406 \text{ mol O}$$

3. we arrive at the formula $C_{3.407}H_{4.54}O_{3.406}$, divide all the subscripts by the smallest subscript ٣.٤٠٦

4. This gives $CH_{1.33}O$ as the formula for ascorbic acid. Next, we need to convert 1.33, the subscript for H, into an integer. This can be done by multiply all the subscripts by 3 and obtain the empirical formula for ascorbic acid as:

$$C_3H_4O_3$$

Problem 2

- **A 1.261 g sample of Caffeine was analyzed to see that it have 0.624 g C, 0.065 g H, 0.364 g N and 0.208 g O. what is the empirical formula of caffeine?**

1. we need to convert the grams of each element to moles:

   $n = m/M$

   $n_C = 0.624/12.01 = 0.052$ mol C

   $n_H = 0.065/1.008 = 0.065$ mol H

   $n_N = 0.364/14.0 = 0.026$ mol N

   $n_O = 0.208/16.00 = 0.0130$ mol O

2. we arrive at the formula $C_{0.052}H_{0.065}N_{0.026}O_{0.0130}$, divide all the subscripts by the smallest subscript 0.0130.
3. This gives $C_4H_5N_2O$ as the formula for caffeine.

Problem 3

- **Suppose that in one experiment the combustion of 11.5 g of a compound (contain C, H and O) produced 22.0 g of CO2 and 13.5 g of H2O. Calculate the empirical formula of the compound?**

$$1 \text{ mole of } CO_2 \;\hat{=}\; 1 \text{ mole of } C$$
$$22/44 \text{ mol} \;\hat{=}\; ??$$

- $n_C = 0.5$ mol So, $m_C = 0.5 \times 12 = 6$ g

$$1 \text{ mole of } H_2O \;\hat{=}\; 2 \text{ mole of } H$$
$$13.5/18 \text{ mol} \;\hat{=}\; ??$$

- $n_H = 1.5$ mol So, $m_H = 1.5 \times 1 = 1.5$ g
- Then,

$$\begin{aligned} \text{mass of O} &= \text{mass of sample} - (\text{mass of C} + \text{mass of H}) \\ &= 11.5 \text{ g} - (6.00 \text{ g} + 1.51 \text{ g}) \\ &= 4.0 \text{ g} \end{aligned}$$

- $n_O = 4/16 = 0.25$ mol
- So,

$C_{0.50}H_{1.5}O_{0.25}$ divide the subscripts by 0.25, C_2H_6O

Determination of Molecular Formulas from empirical formula

Steps

- The formula calculated from elemental analysis is always the empirical formula.
- To calculate the actual, molecular formula we must know the *approximate* molar mass of the compound experimentally.
- The integral relationship between the empirical and molecular formulas could be obtained from the following ratio:

$$\text{No. of folds} = \frac{\text{molar mass}}{\text{empirical molar mass}}$$

- Molecular formula = No. of folds *(empirical formula)

Problem 3

- From problem 2, calculate the molecular formula of caffeine if you know that its molar mass ≈ 194.19 g/mol?

1. Empirical molar mass of $C_4H_5N_2O$ = 97 g/mol
2. No. of folds = $\frac{\text{molar mass}}{\text{empirical molar mass}}$

   = 194.19/97 ≈ 2
3. Molecular formula = 2 (empirical formula)
4. Molecular formula is $C_8H_{10}N_4O_2$

Chemical Reactions and Chemical Equations

Definitions

- A **chemical reaction**, a process in which a substance (or substances) is changed into one or more new substances.

- A **chemical equation** uses chemical symbols to show what happens during a chemical reaction.

Writing Chemical Equations

- For the following reaction:

$$2H_2 + O_2 \longrightarrow 2H_2O$$

1. The “plus” sign means “reacts with” and the arrow means “to yield.”
2. We refer to H2 and O2 in the Equation as reactants, and Water is the product.
3. **Reactants,** are the starting materials in a chemical reaction and written on the left of the arrow.
4. **Products**, are the substances formed as a result of a chemical reaction and written on the right of the arrow.

5. Chemists often indicate the physical states of the reactants and products by using the letters *g*, *l*, and *s* to denote gas, liquid, and solid, respectively. *aq* denotes the aqueous (that is, water) environment.

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$
$$2HgO(s) \longrightarrow 2Hg(l) + O_2(g)$$

$$NaCl(s) \xrightarrow{H_2O} NaCl(aq)$$

TABLE 3.1	Interpretation of a Chemical Equation		
$2H_2$	$+ O_2$	$\longrightarrow$	$2H_2O$
Two molecules	+ one molecule	$\longrightarrow$	two molecules
2 moles	+ 1 mole	$\longrightarrow$	2 moles
$\underbrace{2(2.02\ g) = 4.04\ g + 32.00\ g}_{36.04\ g\ \text{reactants}}$		$\longrightarrow$	$\underbrace{2(18.02\ g) = 36.04\ g}_{36.04\ g\ \text{product}}$

Balancing Chemical Equations

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 to conform with the law of conservation of mass, there must be the same number of each type of atom on both sides of the arrow.
3. We can change the coefficients (the numbers preceding the formulas) but not the subscripts (the numbers within formulas).
4. 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.
5. Next, look for elements that appear only once on each side of the equation but in unequal numbers of atoms. Balance these elements.
6. Finally, balance elements that appear in two or more formulas on the same side of the equation.
7. 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.

Example 1

- Small amounts of oxygen gas can be prepared by heating potassium chlorate (KClO3). The products are oxygen gas (O2) and potassium chloride (KCl). From this information, we write

$$KClO_3 \longrightarrow KCl + O_2$$

- All three elements (K, Cl, and O) appear only once on each side of the equation, but only for K and Cl do we have equal numbers of atoms on both sides. Thus, KClO3 and KCl must have the same coefficient.
- The next step is to make the number of O atoms the same on both sides of the equation:

$$2KClO_3 \longrightarrow KCl + 3O_2$$

Example 1

- Finally, we balance the K and Cl atoms :

$$2KClO_3 \longrightarrow 2KCl + 3O_2$$

- As a final check the number of atoms on each side for the reactants and products.

Example 2

- The combustion (that is, burning) of the natural gas component ethane (C2H6) in oxygen or air, yields carbon dioxide (CO2) and water. The unbalanced equation is:

$$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$$

- We see that the number of atoms is not the same on both sides of the equation for any of the elements (C, H, and O). In addition, C and H appear only once on each side of the equation; O appears in two compounds on the right side (CO2 and H2O).
- First, balance the C atoms:

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + H_2O$$

- Then, balance the H atoms:

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + 3H_2O$$

Example 2

- At this stage, the C and H atoms are balanced, but the O atoms are not, so balance them:

$$C_2H_6 + \frac{7}{2}O_2 \longrightarrow 2CO_2 + 3H_2O$$

- However, we normally prefer to express the coefficients as whole numbers rather than as fractions. Therefore, we multiply the entire equation by 2 to get:

$$2C_2H_6 + 7O_2 \longrightarrow 4CO_2 + 6H_2O$$

- As a final check the number of atoms on each side for the reactants and products.

Amounts of Reactants and Products

The mole method

- A basic question raised in the chemical laboratory is “How much product will be formed from specific amounts of reactants?”.
- Or in some cases, we might ask the reverse question: “How much reactants must be used to obtain a specific amount of product?”
- For example, the combustion of carbon monoxide in air produces carbon dioxide:

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

- This equation can 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 CO2, that is,

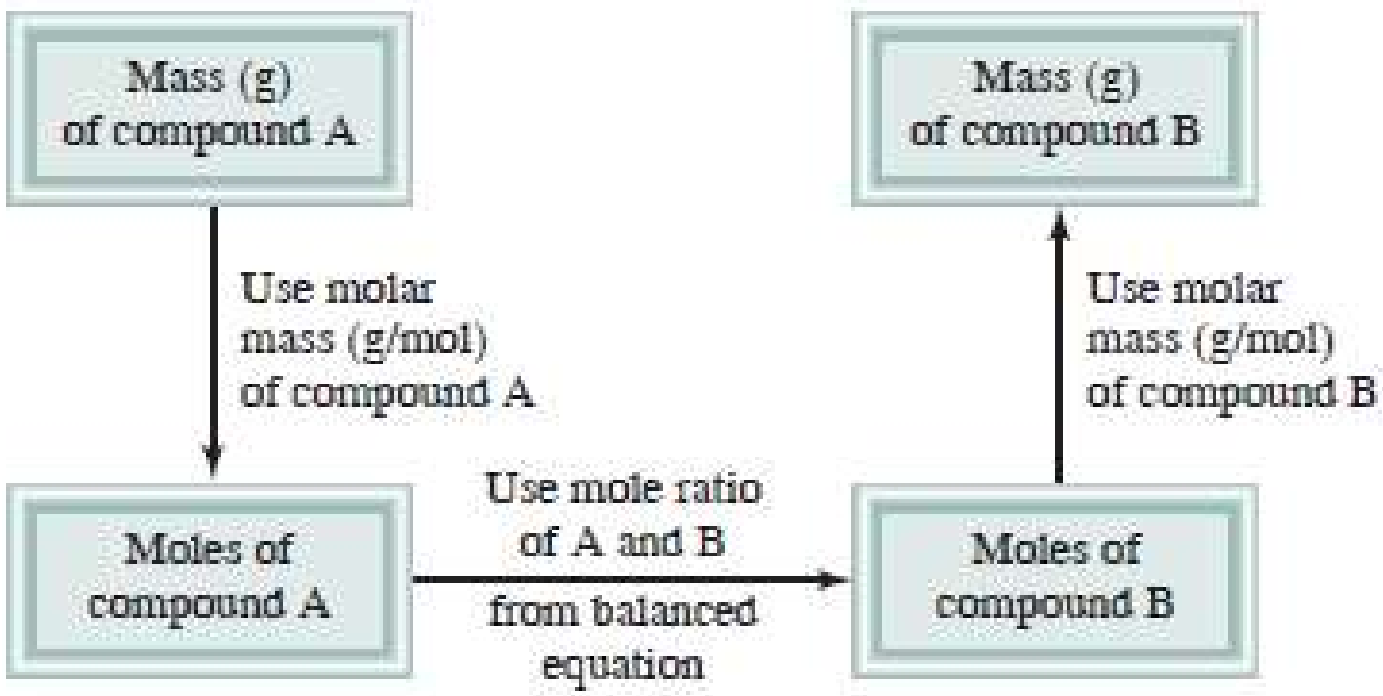
$$2 \text{ mol CO} \mathrel{\hat{=}} 2 \text{ mol } CO_2$$

- where the symbol $\hat{=}$ means “stoichiometrically equivalent to” or simply “equivalent to.”
- Similarly, we have 1 mol O2 $\hat{=}$ 2 mol CO2 and 2 mol CO $\hat{=}$ 1 mol O2.

The mole method

- The mole method used to calculate the amount of reactants or products in a chemical reaction by their molar ratios.
- First convert the quantity of reactant A (in grams or other units) to number of moles.
- Next, use the mole ratio in the balanced equation to calculate the number of moles of product B formed.
- Finally, convert moles of product to grams of product.
- If the grams of the products are given to calculate the grams of the reactants, do the same procedure above.

Summary for the mole method



Example

- **A general overall equation for the degradation of glucose ($C6H12O6$) to carbon dioxide ($CO2$) and water ($H2O$):**

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

If 856 g of $C6H12O6$ is consumed by a person over a certain period, what is the mass of $CO2$ produced?

1. From the equation:

   1 mole of $C6H12O6$ ≏ 6 moles of $CO2$

2. no. of moles of $C6H12O6$ (n)= mass (m)/ molar mass(M)

   = 856/ 180= 4.750 mol $C6H12O6$

3. no. of moles of C= 4.750 X 6 = 28.50 mol $CO2$
4. Mass of $CO2$ (m) = n*M= 28.5 X 44 = 1.25 X 10^3 g $CO2$

Limiting Reagents

Definitions

- When a chemist carries out a reaction, the reactants are usually not present in exact stoichiometric amounts indicated by the balanced equation.
- Because the goal of a reaction is to produce the maximum quantity of a useful compound from the reactants, 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 (finished) first in a reaction is called the **limiting reagent**.
- **Excess reagents** are the reactants present in quantities greater than necessary to react with the quantity of the limiting reagent.
- In practice, chemists usually choose the more expensive chemical as the limiting reagent so that all or most of it will be consumed in the reaction.

Calculations

- In stoichiometric calculations involving limiting reagents, the first step is to decide which reactant is the limiting reagent.
- **How to determine the limiting reagent?**

1. Calculate the no. of moles for each reactant from the data given.
2. For each reactant, divide the no. of moles calculated from step 1 by the no. of moles indicated in the balanced equation.
3. Compare the two ratios obtained from step 2, the smallest ratio is for the limiting reagent.

- After the limiting reagent has been identified, the rest of the problem can be solved as outlined in the mole method.

Problem

- **Urea $[(NH_2)_2CO]$ is prepared by reacting ammonia with carbon dioxide:**

$$2NH_3(g) + CO_2(g) \longrightarrow (NH_2)_2CO(aq) + H_2O(l)$$

- **In one process, 637.2 g of NH_3 are treated with 1142 g of CO_2.**

  (a) Which of the two reactants is the limiting reagent?

  (b) Calculate the mass of $(NH_2)_2CO$ formed.

  (c) How much excess reagent (in grams) is left at the end of the reaction?

  Solution for a:

1. No. of moles of NH_3 = m/M= 637.2/17.03= 37.42 mol

   No. of moles of CO_2 = m/M= 1142/44= 25.95 mol

2. For NH_3, 37.42/2= 18.71

   For CO_2, 25.95/1= 25.95

3. As 18.71 is smaller than 25.95, so NH_3 is the limiting reagent.

- **Solution for b:**
- Use the mole method and regarding that NH_3 is the limiting reagent

1. From the equation:

   2 mole of NH_3 $\triangleq$ 1 mole of $(NH_2)_2CO$

2. no. of moles of NH_3 reacted in equation = 37.42 mol
3. no. of moles of $(NH_2)_2CO$= 37.42/2= 18.71 mol
4. Mass of $(NH_2)_2CO$ = n*M= 18.71 X 60.06 = 1124 g

- **Solution for c:**

1. From the equation:

   2 mole of NH_3 $\hat{=}$ 1 mole of reacted CO_2

2. no. of moles of NH_3 reacted in equation = 37.42 mol
3. no. of moles of reacted CO_2= 37.42/2= 18.71 mol
4. Mass of reacted CO_2 = n*M= 18.71 X 44 = 823.24 g
5. Mass of excess CO_2= 1142-823.24= 318.76 g

Reaction Yield

Definitions

- The amount of limiting reagent present at the start of a reaction determines the theoretical yield of the reaction.
- **Theoretical yield** is the maximum amount of product that would result if all the limiting reagent reacted.
- In practice, the actual yield is almost always less than the theoretical yield.
- **Actual yield** is the amount of product actually obtained from a reaction.
- To determine how efficient a given reaction is, chemists often figure the percent yield.
- **Percent yield** describes the proportion of the actual yield to the theoretical yield. It is calculated as follows:

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

Problem

- From the previous problem, if you know that actual yield of urea is 1000 g, calculate the reaction yield?

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

= 1000/1124 X 100% = 89%