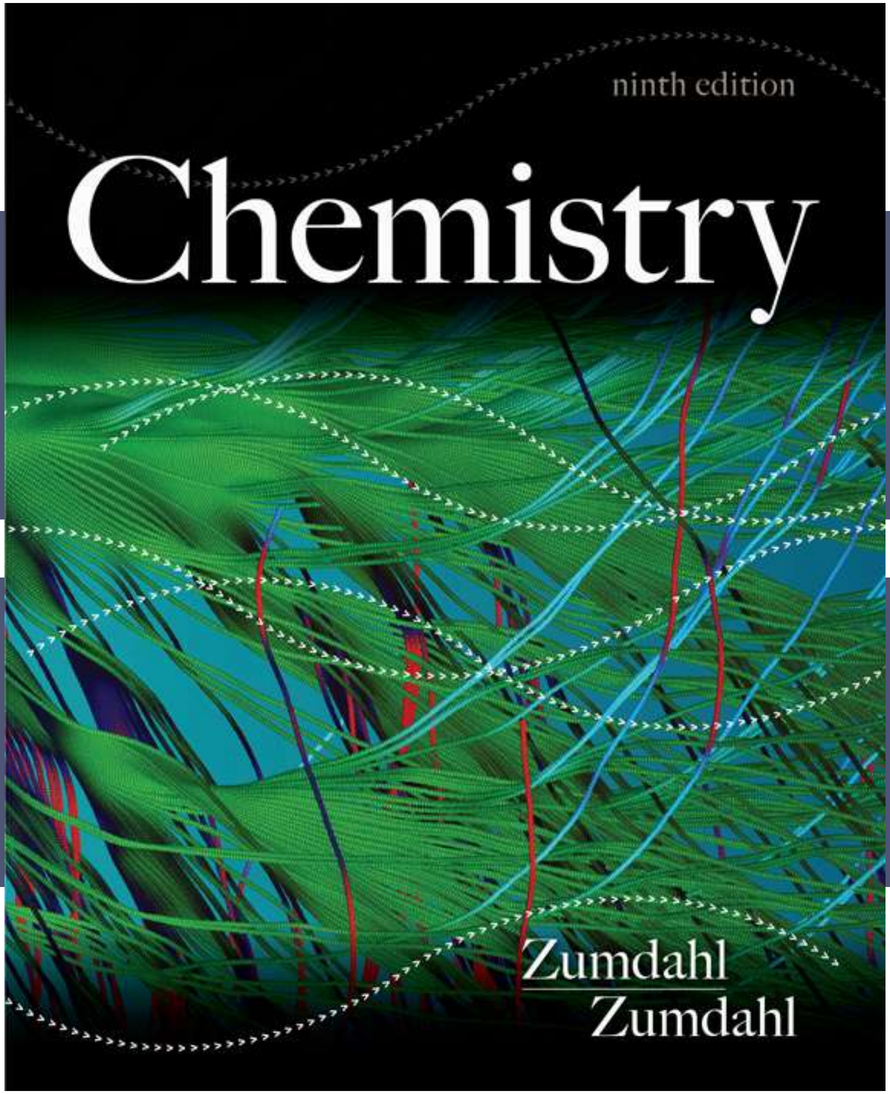


Chapter 3

Stoichiometry

Chemical Stoichiometry

- Definition of Stoichiometry:

  Chemical calculations.

  Calculating the amounts (moles and masses) of reactants and products in chemical reactions.

- <u>Average</u> mass of an object.
- ^{12}C is the reference for atomic masses. Its atomic mass is exactly 12 atomic mass units (a.u).
- The masses of all other atoms are given relative this mass of ^{12}C.
- The ratio of the mass of an isotope to that of ^{12}C is found by an instrument called <u>mass spectrometer</u>.
- Elements occur in nature as mixtures of isotopes.
- Carbon : 98.89% ^{12}C

  1.11% ^{13}C

  < 0.01% ^{14}C

Atomic mass of an isotope from data obtained from mass spectrometer:

- Mass spectrophotometer gives mass ratio of an isotope to that of ^{12}C.
- Calculate the mass of ^{13}C if its mass ratio to that of ^{12}C is 1.08362?

Solution:

Mass of ^{12}C = 12 a.u *(the reference for atomic masses)*

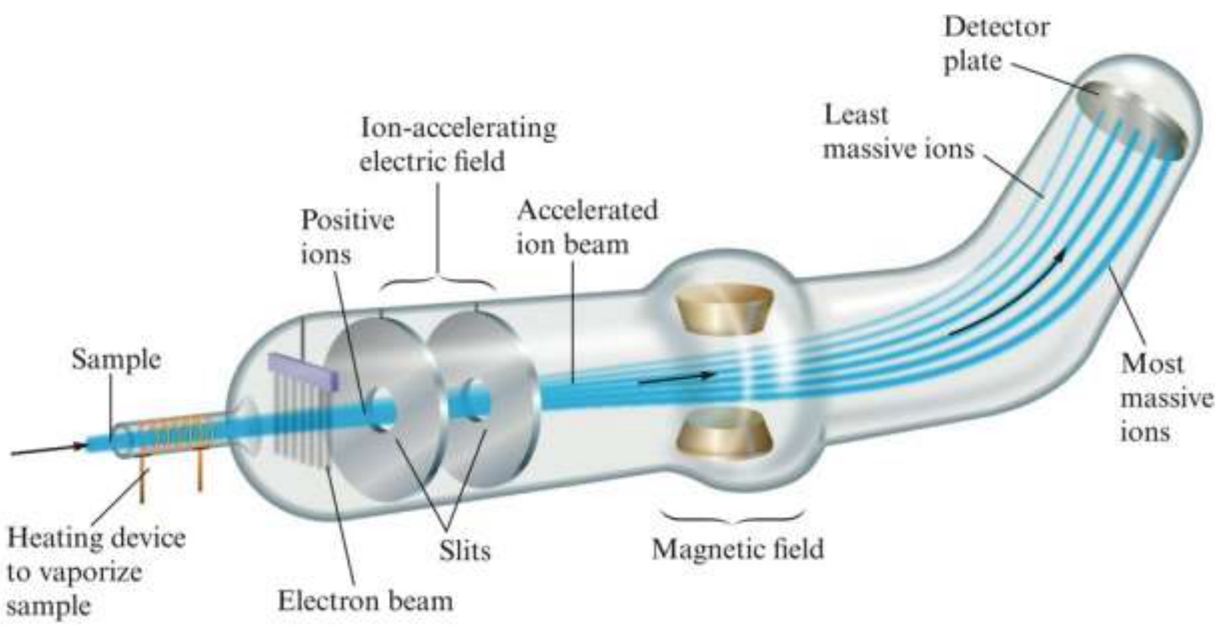
From mass spectrometer: mass $^{13}C/^{12}C = 1.08362$

So, mass of ^{13}C = (mass of ^{12}C)(1.08362)

= (12 a.u)(1.08362) = 13.0034 a.u

Schematic Diagram of a Mass Spectrometer

Geoff Tompkinson/Photo Researchers, Inc.



Average Atomic Mass for Carbon:

From mass spectrometer, ratio $^{13}C/^{12}C = 1.08362$

Use the following data to calculate the average atomic mass of carbon:

^{12}C	98.89%	12 a.u
^{13}C	1.11%	1.08362
^{14}C	< 0.01%	*(very small so: neglected)*

average atomic mass = Σ (atomic mass)(aboundancy) ; (for all isotopes)

= (12 a.u) (0.9889)+ (13.0034 a.u)(0.0111) = 12.01 a.u

<u>NOTE</u>: ^{14}C is neglected (< 0.01%)

Average Atomic Mass for Carbon **(SKIP)**

- Even though natural carbon does not contain a single atom with mass 12.01, for stoichiometric purposes, we can consider carbon to be composed of only one type of atom with a mass of 12.01.
- Example on averages:

  Marks: 84, 81, 75 the average is 80, it is used to represent the mark for the semester even though none of the grades is 80.

Section 3.3
The Mole

- 1 mole of substance is 6.022×10^{23} units of that substance (Avogadro's number).
- 1 mole C = 6.022×10^{23} C atoms = 12.01 g C
- 1 mole of any element contains $6.022x10^{23}$ atoms and its mass is the atomic mass of the element.
- The number of atoms can be calculated from the number of moles.
- Number of moles (n) can be calculated from the mass and the atomic mass,
- n = mass/atomic mass
- $1\ mol\ of\ an\ element = 6.022x10^{23}\ atoms = atomic\ mass$
- $1\ mole\ of\ a\ compound = 6.022x10^{23}\ molecules = malar\ mass$

Calculate the number of moles of iron in a 23.25 g iron?

n = mass/atomic mass

= 23.25/55.85 g/mole = 0.416 mol.

Exercise: calculate the number of atoms?

Answer: 2.51×10^{23} Fe atoms

- Mass in grams of one mole of the substance:

  Atomic Mass of N = 14.01 g/mol.

  Molar Mass of H_2O = 18.02 g/mol.

  $(2 \times 1.008\ g) + 1x16.00\ g = 18g/mol.$

  n = mass/MM ; n = mass/atomic mass

  Molar Mass of $Ba(NO_3)_2$ = 261.35 g/mol.

  $137.33\ g + (2 \times 14.01\ g) + (3x2 \times 16.00\ g)$

  N_2 : $MM(N_2)$= 2x14.01 =....

- Mass percent of an element:

$$\text{mass }\% = \frac{\text{mass of element in compound}}{\text{mass of compound}} \times 100\%$$

- Basis: 1 mole of the compound
- Iron in iron(III)oxide, (Fe_2O_3):

MM (Fe_2O_3) = 2(55.85 g) + 3(16.00 g) = 159.70 g/mol

Mass of Fe in 1 mole of Fe_2O_3 = 2(55.85 g) = 117.70 g

So, mass % Fe = [117.70/159.70] x 100% = 69.94%

% O = 100% – 69.94% = 30.06 %

Exercise: how many grams of oxygen are in 45.7 g of a sample of Fe_2O_3?

$$1C_2H_5OH + 3O_2 \longrightarrow 2CO_2 + 3H_2O$$

- 1 mole of ethanol reacts with 3 moles of oxygen to produce 2 moles of carbon dioxide and 3 moles of water.
- The equation is balanced.
- The number of atoms of each element in the reactants and products are equal.
- Exercise: calculate the mass percent of ethanol (C_2H_5OH)?

Balance the following equation?

$$2\,CaO + 5C \longrightarrow 2\,CaC_2 + CO_2$$

$$CaO + 2.5\,C \longrightarrow CaC2 + 0.5CO2$$

CaO: 2 C: 5 CaC_2: 2 CO_2: 1

Stoichiometric Coefficients

Notice

- The number of atoms of each type of element must be the same on both sides of a balanced equation.
- Subscripts must <u>not</u> be changed to balance an equation.
- A balanced equation tells us the number of <u>moles</u> of each of the reactants and products.
- Coefficients can be fractions, although they are usually given as <u>lowest integer multiples</u>.

Stoichiometric Calculations

- In chemical calculations, balanced chemical equations are used to relate any reactants and products together, or any reactants alone together, or any products alone together. The relation can be mole relation, or mass relation or mixed (moles and masses) relation. This will be illustrated with examples.

- Stoichiometric Coefficients

Calculating Masses of Reactants and Products in 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.

Section 3.10
Stoichiometric Calculations: Amounts of Reactants and Products

- To do any stoichiometric calculations

  We need the MM and the stoichiometric coefficients to build up the relations that we need.

- Consider the following reaction:

MM (g/mol.): $N_2 = 28$; $H_2 = 2$; $NH_3 = 17$

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

1 mol.	3 moles	2 moles
1x28 g	3x2 g	2x17 g
28 g	6 g	34 g
0.1 mol		

How many grams of ammonia are produced when 0.25 mol. of nitrogen reacted with sufficient amount of hydrogen?

Answer: 0.25x2x17 = 8.5g

Section 3.10
Stoichiometric Calculations: Amounts of Reactants and Products

Consider the following reaction:

$$P_{4\,(s)} + 5O_{2\,(g)} \rightarrow 2P_2O_{5\,(s)}$$

How many <u>grams</u> and <u>moles</u> of oxygen are required to react with 6.25 g of phosphorous, P_4? n=mass/MM

MM (g/mol.): P_4 = 123.9; O_2 = 32.0; P_2O_5 = 141.94.

Moles of phosphorous (P_4) = 6.25g/123.9 g/mol. = 0.0504 mol.

Moles of O_2 = 5 x moles of P_4 = 5 x 0.0504 = 0.252 mol.

Mass of O_2 = moles x MM = 0.252 x 32 = 8.064 g.

Exercise: Calculate moles and mass of P_2O_5 produced?

Answer: Moles = 0.1008 mol. Mass = 14.31 g

<u>Important Note</u>: in chemical reactions mass is conserved.
ALWAYS: mass of reactants = mass of products.

Exercise:

Methane (CH_4) and ammonia (NH_3) react with oxygen according to the reactions below:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
$$4NH_3 + 7O_2 \rightarrow 4NO_2 + 6H_2O$$

I) How many moles of water are produced when 1.0 g CH_4 reacted with sufficient oxygen?

II) What mass of ammonia required to react with sufficient oxygen to produce the same amount of water in part (I)?

Answer: (I) 0.125 mole of water are produced.

(II) 1.416 g of ammonia are required.

MM (g/mol.): CH_4 = 16; H_2O = 18; NH_3= 17.

Limiting Reactants

- Limiting reactant – the reactant that runs out first and thus limits the amounts of products that can be formed.
- Determine which reactant is limiting to calculate correctly the amounts of products that will be formed.

Example: (Stoichiometric and none-stoichiometric mixing)

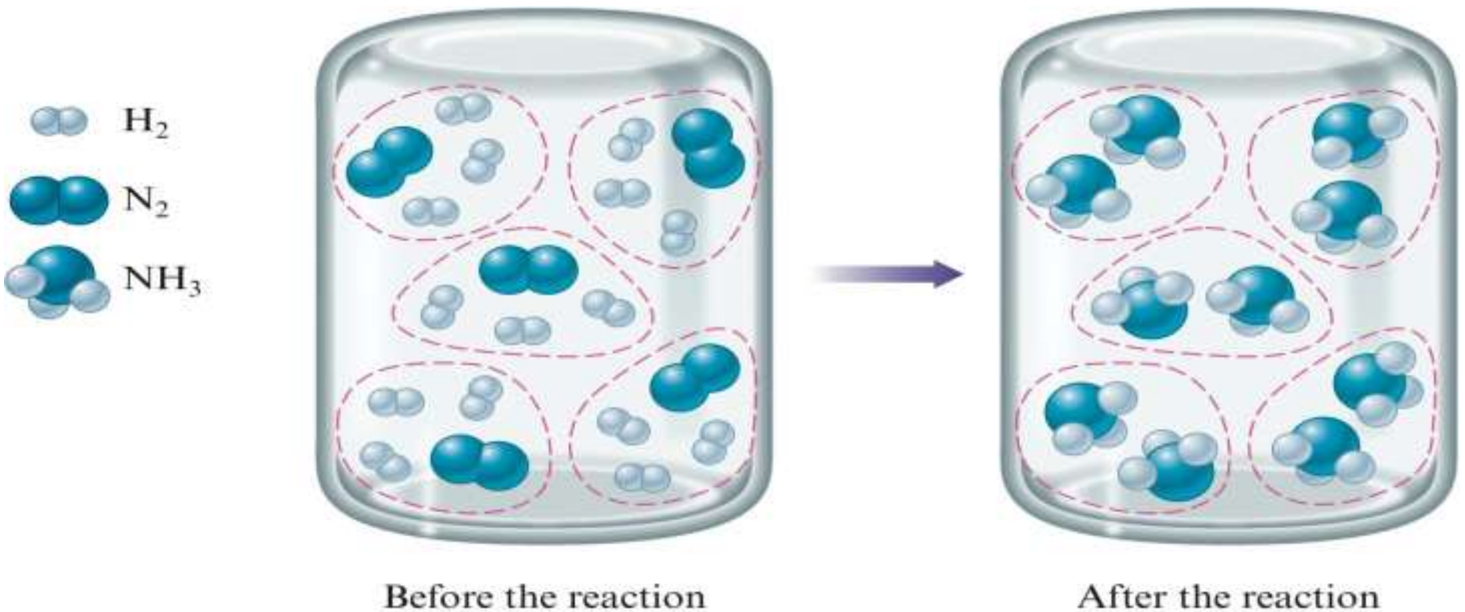
1:1	$CH_{4\,(g)}$ +	$H_2O_{(g)}$ →	$3H_{2\,(g)}$ +	$CO_{(g)}$	
	1.0	1.0	3.0	1.0	SM
	0.5	0.5	1.5	0.5	SM
	1.0	2.0	3.0	1.0	NSM
	5.0	2.0	6.0	2.0	NSM

3:1		$3H_{2\,(g)}$	+	$N_{2\,(g)}$	$\rightarrow$	$2NH_{3\,(g)}$		
		3 mol.		1 mol.		2 mol.		
		1.5		0.5		1.0		
		5		2		3.33		
		4		1		2.00		
2:3	$2CH_4$	+	$3O_2$		$\rightarrow$	$2CO$	+	$4H_2O$
	2		3			2		4
	1		2			1		2
	3		4			?		?

Moles can be converted into masses and vice versa

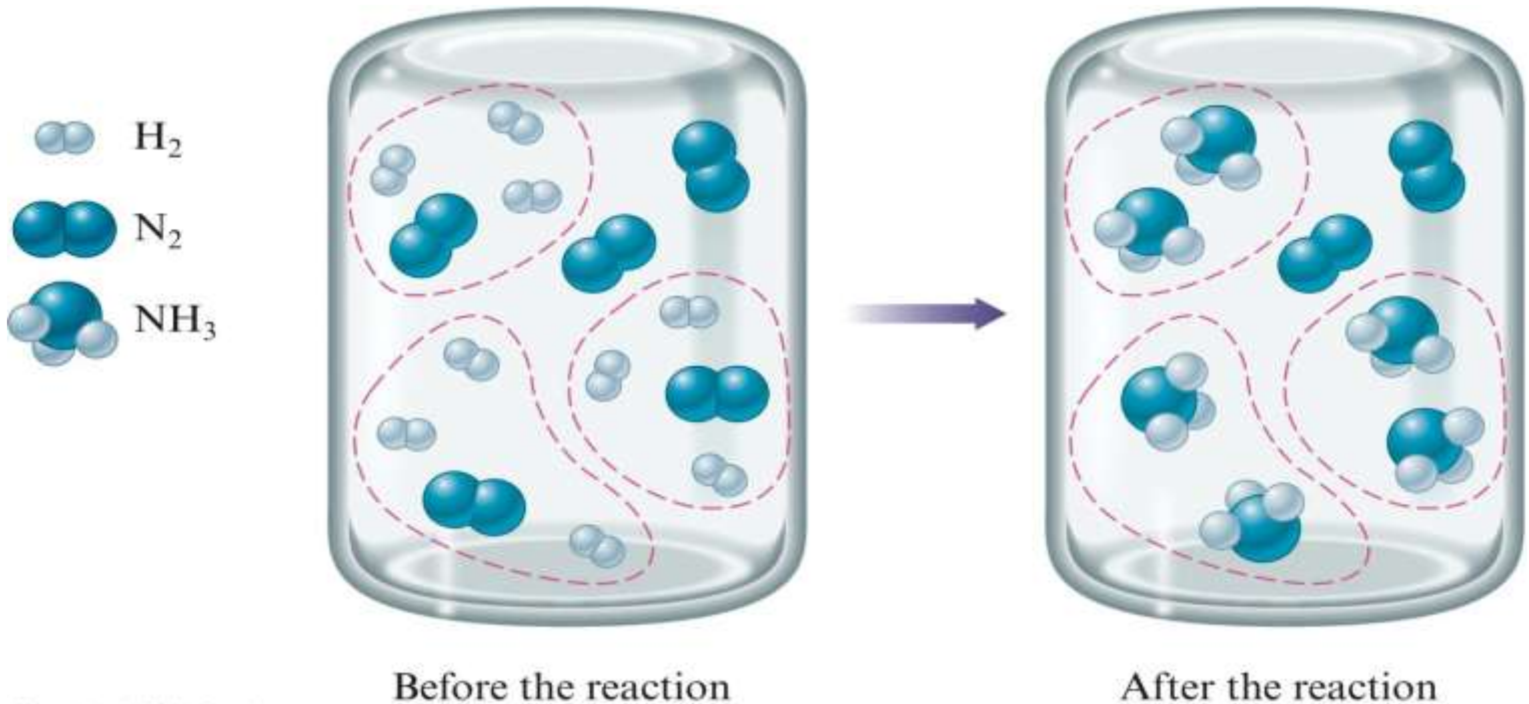
A. Stoichiometric mixing: (all reactants are consumed and converted into products)

$$N_{2\,(g)} + 3H_{2\,(g)} \rightarrow 2NH_{3\,(g)}$$



B. None-stoichiometric mixing: (Limiting reactant)

$$N_{2\,(g)} + 3H_{2\,(g)} \rightarrow 2NH_{3\,(g)}$$



- The Limiting Reactant (L.R):
  - L.R. happens when the mixing is none-stoichiometric.
  - The L.R runs out from the reaction mixture first
  - When the reaction is 1:1, the L.R is the reactant with lower number of moles.
  - When the reaction is not 1:1, then simple calculation is needed to find out the L.R.

All Calculations Are Based On The L.R.

Consider the reaction between methane gas and water;

$$CH_{4\,(g)} + H_2O_{(g)} \rightarrow 3H_{2\,(g)} + CO_{(g)}$$

Calculate the mass of H_2 produced when 2.5 moles of CH_4 are mixed with 31.5 g of H_2O? MM(CH_4) = 16; H_2O = 18; H_2 = 2.

[Mixing of reactants so we should think of L.R]

n (CH_4) = 2.5 mol.

n (H_2O) = mass/MM = 31.5 g/18 g/mol. = 1.75 mol.

The ratio of the reactants is 1:1, so, the substance with lower number of moles is the L.R, it is H_2O.

Remeber:

$\boxed{\text{All Calculations Are Based On The L.R.}}$

Since H_2O is the L.R,

moles of H_2 produced = 3 (moles of H_2O reacted)

= 3(1.75) = 5.25 mol.

Mass of H_2 produced = (n)(MM) = (5.25 mol.)(2 g H_2 /mol.)

= $\boxed{\text{10.5 g } H_2 \text{ produced.}}$

How many <u>moles</u> of CO are produced? 1.75 mol.

How many <u>grams</u> of CO are produced? 49 g

How many grams of CH_4 reacted? ?

How many grams of CH_4 unreacted? ?

Percentage Yield

- An important indicator of the efficiency of a particular laboratory or industrial reaction.
- Theoretical yield is obtained by calculation.
- Actual yield is obtained experimentally.

$$\boxed{\frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\% = \text{percent yield}}$$

- Consider the reaction: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Calculate the percentage yield if 72.3 g of water are produced when 45 g of methane gas react with sufficient amount of oxygen?

MM(g/mol.): CH_4 = 16; H_2O = 18

[Note: explain to the students that there is no L.R in this question]

Theoretical yield:

n (CH_4) reacted = mass/MM = 45g/16 = 2.81 mol.

n (H_2O) produced = 2xn(CH_4) reacted = 2(2.81) = 5.62 mol.

Mass of H_2O produced = (n) MM = (5.62)(18) = 101.2 g.

% yield = [Actual y./Theoretical y.] 100%

= (72.3 g/101.2 g)(100%) = $\boxed{71.44\ \%}$

Consider the following reaction: *(Homework)*

$$P_{4\,(s)} + 6F_{2\,(s)} \rightarrow 4PF_{3\,(g)}$$

What <u>mass</u> of P_4 is needed to produce 85.0 g of PF_3 if the reaction is 64.9% yield?

MM(g/mol): P_4 = 123.89 , PF_3 = 87.97

Answer: Mass of P_4 required = $\boxed{46.1\text{ g}}$