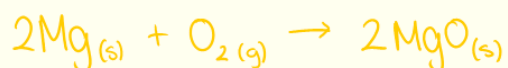


1.4 – Mass and Gaseous Volume Relationships in Chemical Reactions

1.4.1 - Calculate theoretical yields from chemical equations

A balanced equation establishes the connection between the mass (or moles) of a known substance to the mass (or moles) of an unknown substance.

For example:



We have: 2.431g Mg and excess O_2

$$n(\text{Mg}) = \frac{m}{M} = \frac{2.431}{24.31} = 0.1000 \text{ mol}$$

The ratio of Mg to MgO is 2:2, or 1:1

$$n(\text{MgO}) = \frac{1}{1} \times n(\text{Mg}) = \frac{1}{1} \times 0.1000 = 0.1000 \text{ mol MgO}$$

$$m(\text{MgO}) = n \times M = 0.1000 \times 40.31 = 4.031 \text{ g}$$

Calculations like this can be done in the following steps:

- ① Write a balanced chemical equation
- ② List the given data with units, and a symbol.
i.e. $n = 0.20 \text{ mol}$
 $m = 4.72 \text{ g}$
 $V = 30 \text{ dm}^3$
- ③ Convert the data for the known quantity to moles, using:
 $n = \frac{m}{M}$ $n = cV$ $n = \frac{N}{L}$ $n = \frac{V}{V_m}$ $n = \frac{PV}{RT}$
- ④ Find the molar ratio between the known and unknown quantities and calculate the number of moles of the unknown
- ⑤ Convert back to the relevant units



1.4.2 - Determine the limiting reactant in excess when quantities of reacting substances are given

If there is more than one reactant, the **limiting reactant** needs to be identified. We determine the amount (in moles) of both reactants and use the molar ratio to from the equation to determine which will be completely consumed in the reaction and which is present in excess. The limiting reagent is the one used in the calculation.

① Write the equation:



② List relevant data

$$\begin{array}{lll} m(\text{C}) = 40.0\text{g} & m(\text{SiO}_2) = 40.0\text{g} & m(\text{SiC}) = x \\ M(\text{C}) = 12.01\text{ g mol}^{-1} & M(\text{SiO}_2) = 60.09\text{ g mol}^{-1} & M(\text{SiC}) = 40.10\text{ g mol}^{-1} \end{array}$$

③ Convert everything into moles

$$n(\text{C}) = \frac{40.0}{12.01} = 3.331\text{ mol} \quad n(\text{SiO}_2) = \frac{40.0}{60.09} = 0.6657$$

④ Determine the excess reagent

$$\begin{array}{l} \text{C} : \text{SiO}_2 \\ 2 : 1 \end{array} \quad \therefore \quad \frac{1}{2} \times 3.331\text{ mol C} = 1.666\text{ mol C} \leftarrow \text{excess}$$

$$\frac{1}{1} \times 0.6657\text{ mol SiO}_2 = 0.6657\text{ mol SiO}_2$$

C is in excess and SiO₂ is the limiting reactant

Find the molar ratio between the LR and unknown quantity

$$\begin{array}{l} \text{SiO}_2 : \text{SiC} \\ 1 : 1 \end{array} \quad \therefore \quad n(\text{SiO}_2) = n(\text{SiC}) = 0.6657\text{ mol}$$

⑤ Convert to the relevant units

$$n(\text{SiC}) = 0.6657 \times 40.10 = 26.69\text{g}$$



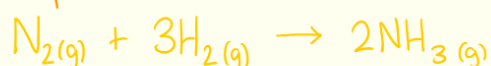
1.4.3 - Solve problems involving theoretical, experimental and percentage yield

The amount of product produced in an experiment is called the experimental yield. It is often significantly less than the theoretical yield. To express how successful the preparation of a product has been, you calculate the percentage yield.

$$\text{Percentage Yield} = \frac{\text{experimental yield}}{\text{theoretical yield}} \times \frac{100}{1}$$

Example: Haber Process

- ① Write the equation



- ② List given data

$$m(\text{N}_2) = 42.03\text{g}$$

excess H_2

$$m(\text{NH}_3) = x$$

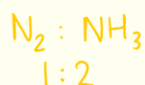
$$M(\text{N}_2) = 28.02 \text{ g mol}^{-1}$$

$$M(\text{NH}_3) = 17.04 \text{ g mol}^{-1}$$

- ③ Convert to moles

$$n(\text{N}_2) = \frac{m}{M} = \frac{42.03}{28.02} = 1.500 \text{ mol N}_2$$

- ④ Find the molar ratio of known and unknown



$$1 : 2$$

$$n(\text{NH}_3) = \frac{2}{1} \times n(\text{N}_2) = 3.000 \text{ mol}$$

- ⑤ Convert to relevant units

$$m(\text{NH}_3) = nM = 3.000 \times 17.03 = 51.12\text{g}$$

* This is the theoretical yield

- ⑥ Calculate the percentage yield.

$$\text{Experimental yield} = 45.00\text{g}$$

$$\text{Theoretical yield} = 51.12\text{g}$$

$$\text{Percentage yield} = \frac{45.00\text{g}}{51.12\text{g}} \times 100 = 88.0\%$$



1.4.4 - Apply Avogadro's law to calculate reacting volumes of gases

Avogadro's law is that equal volumes of gases at the same temperature and pressure contain equal numbers of particles. It can be expressed mathematically as:

$$V = kn$$

V = volume
 k = constant
 n = number of particles

For example:

$$\begin{array}{ll} V_1 = 50.0 \text{ dm}^3 & V_2 = x \\ n_1 = 0.00200 \text{ mol} & n_2 = 0.00375 \text{ mol} \end{array}$$

$$\text{Avogadro's Law} = \frac{V_1}{n_1} = \frac{V_2}{n_2} \quad \therefore V_2 = \frac{V_1}{n_1} \times n_2$$

$$\begin{aligned} x &= \frac{50.0}{0.00200} \times 0.00375 \\ &= 93.8 \text{ cm}^3 \end{aligned}$$

1.4.5 - Apply the concept of molar volume at standard temperature and pressure in calculations

For example, if we have 1.00 mol of an ideal gas at 273K (0°C) and 1.0 atm (101.3 kPa). We can calculate the volume of the gas at these conditions using the ideal gas equation:

$$V = \frac{nRT}{P} = \frac{1.00 \times 8.31 \times 273}{101.3} = 22.4 \text{ dm}^3$$

This is the molar volume (V_m) of the gas under the specified conditions.

A gas will always expand to fill any container, so it is pointless to specify a gas volume without specifying its temperature and pressure.



Standard temperature is 0°C

Standard pressure is 1 atm

These are often used when comparing gases.

Many chemical reactions involve gases. We can use these molar volumes (assuming ideal gas behaviour) to carry out stoichiometric calculations.

1.4.6 - Solve problems involving the relationship between temperature, pressure and volume for a fixed mass of an ideal gas

When we use the ideal gas equation, we must ensure that the correct units are used; P in kPa, V in dm³ and T in K

The ideal gas equation defines the behaviour of an ideal gas. Most gases approach this behaviour at low pressures. We can therefore use this equation to determine one gas quantity (i.e. P) if the other three quantities are known (V, T and n).

$$\frac{P_1 V_1}{n_1 T_1} = \frac{P_2 V_2}{n_2 T_2}$$

Where:

P₁ and P₂ = the initial and final gas pressures

V₁ and V₂ = the volumes

T₁ and T₂ = the temperatures

n₁ and n₂ = the amounts of gas

We frequently deal with situations in which the **amount of gas is fixed**. For this fixed amount of gas, the ideal gas equation reduces to what is sometimes called the combined gas law or combined gas equation.

$$n_1 = n_2$$

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$



This equation can be used to solve for any of the six quantities if the other five are known. Remember when using this that the units for P_1 and P_2 must be the same, the units for V_1 and V_2 the same, and temperature must be measured on the Kelvin scale.

For example:

$$\begin{array}{ll} P_1 = 760 \text{ mmHg} & P_2 = 180 \text{ mmHg} \\ V_1 = 95.0 \text{ dm}^3 & V_2 = x \\ T_1 = 297 \text{ K} & T_2 = 284 \text{ K} \end{array}$$

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2} \therefore V_2 = \frac{P_1 V_1 T_2}{T_1 P_2} = \frac{760 \times 95.0 \times 284}{297 \times 180} = 384 \text{ dm}^3$$

1.4.7 - Solve problems using the ideal gas equation, $PV = nRT$

$$\begin{array}{lll} \text{Boyle's Law} & V \propto \frac{1}{P} & \text{at constant } n \text{ and } T \\ \text{Charles' Law} & V \propto T & \text{at constant } n \text{ and } P \\ \text{Avogadro's Law} & V \propto n & \text{at constant } P \text{ and } T \end{array}$$

$$PV = nRT$$

The constant **R** is the universal gas constant. The usual units are:

- P in kPa
- V in dm^3
- T in K
- n in mol

Using these, R becomes $8.31 \text{ J K}^{-1} \text{ mol}^{-1}$



For example:

$$\begin{aligned}P &= 206 \text{ kPa} \\T &= 297 \text{ K} \\R &= 8.31 \text{ J K}^{-1} \text{ mol}^{-1}\end{aligned}$$

$$\begin{aligned}V &= x \\m &= 52.0 \text{ g}\end{aligned}$$

$$PV = nRT \quad n = \frac{m}{M} \quad \therefore PV = \frac{m}{M} RT$$

$$\begin{aligned}V &= \frac{mRT}{PM} \\&= \frac{52.0 \times 8.31 \times 297}{206 \times 44.0} \\&= 14.2 \text{ dm}^3\end{aligned}$$

1.4.8 - Analyse graphs relating to the ideal gas equation

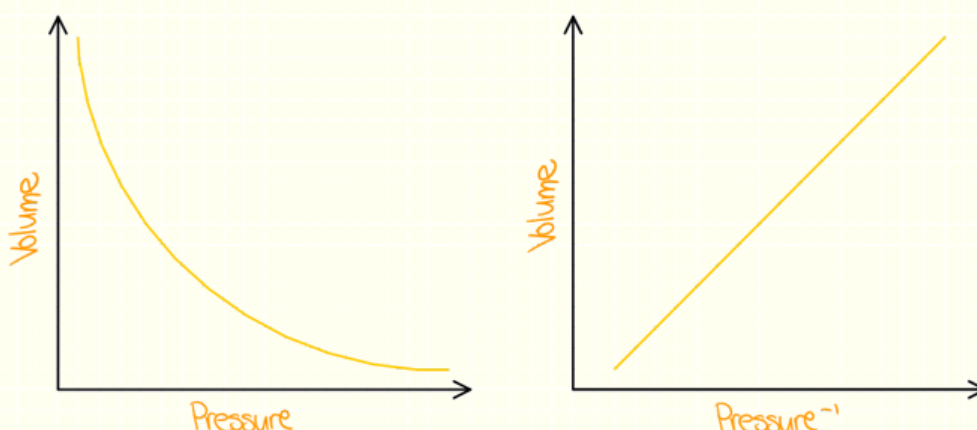
Gas quantities, pressure, volume, amount of gas and temperature are related by a series of mathematical expression known as the gas laws.

Boyle's Law

Boyle studied the relationship between pressure and volume and found that:

The pressure exerted by a given mass of gas at a constant temperature is inversely proportional to the volume occupied by the gas

This relationship can be represented in various ways. A plot of V versus P produces a hyperbola, indicating an inverse relationship. Plotting V versus $1/P$ produces a straight line with an intercept of zero.



This relationship can be represented by the equation:

$$k = PV$$

k is a constant for a given sample of gas at a specified temperature. This can also be shown:

$$P_1V_1 = P_2V_2$$

P_1 = initial pressure

P_2 = final pressure

V_1 = initial volume

V_2 = final volume

This relationship applies provided that the **temperature** and **amount of gas remain constant**. Boyle's law is consistent with the kinetic molecular theory. If the volume of the container is increases, the particles travel greater distances between collisions with each other and the walls of the container. Fewer collisions with the walls mean decreased force per unit area and hence a decreased pressure.

The kinetic molecular theory applies to an **ideal gas**. In an ideal gas the particles are completely independent. Real gases behave less ideally when the pressure is high. Thus, real gases show some deviation from Boyle's law at high pressures. PV is not quite as constant as the pressure increases to values much higher that atmospheric pressure.

For example:

$$P_1 = 750 \text{ mmHg}$$

$$V_1 = 1.2 \text{ dm}^3$$

$$P_2 = 620 \text{ mmHg}$$

$$V_2 = x$$

$$P_1V_1 = P_2V_2 \quad \therefore \quad V_2 = \frac{P_1V_1}{P_2} = \frac{750 \times 1.2}{620} = 1.5 \text{ dm}^3$$

