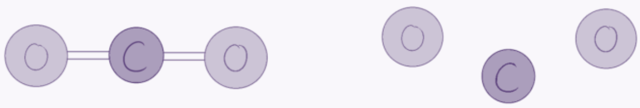
1.1 – The Mole

1.1.1 - Apply the mole concept to substances

A mole is the name given to a certain quantity. It represents 6.02×10^{23} particles. This number is also known as Avogadro's constant, symbolised *L*.

$$L = 6.02 \times 10^{23}\ mol^{-1}$$

To apply this concept to substances, we use it like any other constant. If we have 0.250mol of SO_3 then we would have 0.250mol of S atoms, 0.750mol of O atoms and 1mol of atoms all together.



The mole is used because 6.02×10^{23} particles of anything weigh a certain amount (the molar mass). Exactly 12g of carbon contains 6.02×10^{23} atoms.

1.1.2 - Determine the number of particles and the amount of substance (in moles)

With Avogadro's constant, we can calculate the number of particles present in a given amount of substance.

$$n = \frac{N}{L}$$

where n = number of moles
N = number of particles
L = Avogadro's constant

For example, if we wanted to calculate the number of atoms in 3 moles of Helium, we would do:

$$3mol\ He \times 6.02 \times 10^{23}\ atoms = 1.81 \times 10^{24}\ atoms\ He$$

In reverse, we would do:

$$\frac{1.81 \times 10^{24}\ atoms\ He}{6.02 \times 10^{23}\ atoms} = 3mol\ He$$

You do exactly the same thing if you are asked to calculate the number of ions, molecules, electrons, formula units, etc. For example, if you were asked to find the number of atoms of a certain element in a molecule, then this is what you do:

Find the number of H atoms present in 76.59g of water, H_2O

$$\frac{76.59g\ H_2O}{18.02g\ mol^{-1} H_2O} = 4.25mol\ H_2O$$

$$\text{Since 1mol of water contains 2mol H:}$$

$$2 \times 4.25mol = 8.50mol\ H$$

$$8.50mol\ H\ \times 6.02 \times 10^{23}\ atoms = 5.12 \times 10^{24} atoms\ H$$

$$\therefore \text{in 76.59g of water, there are } 5.12 \times 10^{24} \text{ atoms of hydrogen}$$

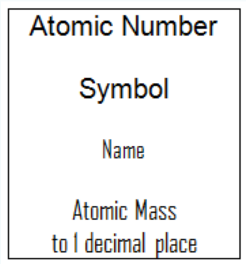
1.2 – Formulas

1.2.1 - Define the terms relative atomic mass (A_r) and relative molecular mass (M_r)

Relative Atomic Mass (A_r) - The weighted mean of the masses of the naturally occurring isotopes, on a scale in which the mass of an atom of the carbon-12 isotope is 12 units exactly.

Relative Molecular Mass (M_r) - The sum of the relative atomic masses of the constituent elements, as given in the molecular formula.

Relative Formula Mass - The same as the Relative Molecular Mass, but it only applies to ionic compounds.



1.2.2 - Calculate the mass of one mole of a species form its formula

The mass of one mole of any substance is equivalent in to its relative atomic (or molecular, or formula) mass, measured in grams.

The mass of one mole of any substance is called the molar mass (M), where the molar mass is equal to the relative atomic mass in units of grams per mole (g mol-1)

For example, if we wanted to find the mass of one mole of HNO_3, we would:

$$\begin{aligned} M_r(HNO_3) &= A_r(H) + A_r(N) + 3A_r(O) \\ &= 1.01 + 14.01 + 3 \times 16.00 \\ &= 63.02 \end{aligned}$$

$$\therefore \text{ one mole of } HNO_3 = 63.02\text{ g}$$

1.2.3 - Solve problems involving the relationship between the amount of substance in moles, mass and molar mass

$$n = \frac{m}{M}$$

n = number of moles
m = mass (g)
M = molar mass ($g\ mol^{-1}$)

For example, if we wanted to find the number of moles there are in 127.1g of copper atoms, we do:

$$127{\cdot}1\,\cancel{g\ Cu} \times \frac{1\ mol\ Cu}{63{\cdot}55\,\cancel{g\ Cu}} = 2{\cdot}000\,mol\ Cu$$

To find the mass of 100 atoms of copper, we do:

$$100\ \cancel{atoms\ Cu} \times \frac{1\,\cancel{mol}}{6{\cdot}02\times10^{23}\,\cancel{atoms}} \times \frac{63{\cdot}55\,g\ Cu}{1\,\cancel{mol}} = 1{\cdot}06\times10^{-20}\,g\ Cu$$

1.2.4 - Distinguish between the terms empirical formula and molecular formula

Empirical Formula - The simplest whole number ratio of atoms of different elements in the compound

Molecular Formula - The actual number of atoms of different elements covalently bonded in a molecule

1.2.5 - Determine the empirical formula from the percentage composition or from other experimental data

There a few simple steps to determining the empirical formula:

① Write the elements present in the compound as a ratio

② Write the percentage composition below each element

③ Divide the percentage by the relative atomic mass of the element, giving a molar ratio

④ Divide each ratio by the smallest one to get a whole-number ratio

⑤ Express the ratios in the empirical formula

1. H : O

2. 11.2% : 88.8%

3. $\div 1.01$ $\div 16.00$
   11.1 : 5.55

4. $\div 5.55$ $\div 5.55$
   $= 2$ $= 1$

5. H_2O

To determine the percentage composition by mass of a compound, given its formula, divide the relative atomic mass of each element present by the relative atomic mass of the compound and express the result as a percentage.

$\boxed{H_2O}$

$$\% H_2 = \frac{H_2}{H_2O} = \frac{2.02}{18.02} = 11.2\%$$

$$\% O = \frac{O}{H_2O} = \frac{16.00}{18.02} = 88.8\%$$

$$\overline{100.0\%}$$

Remember to add all your percentages together at the end to identify any mistakes.

1.2.6 - Determine the molecular formula when given both the empirical formula and experimental data

To determine the **molecular formula**, we must first know the **empirical formula** and the molar mass of the compound. The molar mass of the empirical formula will be in direct proportion to the molar mass of the molecular formula.

For example, if we knew that the empirical formula of a hydrocarbon was CH and its molar mass was 26.04g mol-1, to determine its molecular formula, we would:

$$M(CH) = 13.02\,g\,mol^{-1} \qquad M(\text{compound}) = 26.04\,g\,mol^{-1}$$

$$\frac{M(\text{compound})}{M(\text{empirical formula})} = \frac{26.04}{13.02} = 2$$

So, the molecular formula is 2 times the empirical formula. Therefore, it is: C_2H_2.

1.3 – Chemical Equations

1.3.1 - Deduce chemical equations when all the reactants and products are given

Chemical formulas are shorthand representations of compounds. **Chemical reactions** are represented by equations using the chemical formulas and symbols of the substances involved in the reaction.

methane + oxygen → carbon dioxide + water

$$CH_4 + O_2 \longrightarrow CO_2 + H_2O$$

This equation is more informative than the first. However, when writing out these reactions, we must take into account the Law of Conservation.

The Law of Conservation is that matter can neither be created nor destroyed, it can only be changed from one form into another. In the case of chemical equations, this means that there must be the <u>same number of every type of atom</u> on both sides of the equation. All that happens in a chemical reaction is that the bonds in the reactants break, the atoms rearrange, and bonds between the products are formed. Therefore, to reflect this, all chemical equations must be **balanced**. We do this by adding **integer coefficients** to the chemical formulas, except, of course, in the case of 1.

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

1.3.2 - Identify the mole ratio of any two species in a chemical equation

Once we have balanced any chemical equation, we are able to determine the **molar ratio** of the various species in it. For example:

$$Li_2O_{(s)} + 2HCl_{(aq)} \rightarrow 2LiCl_{(aq)} + H_2O_{(l)}$$

From this equation we can see that one mole of lithium oxide reacts with two mole of hydrochloric acid to produce two mole of lithium chloride and one mole of water.

An equation shows that one mole of gaseous methane molecules combines with two mole of gaseous oxygen molecules, producing one mole of gaseous carbon dioxide and two mole of gaseous water molecules. The equation shows the ratio of reactants and products to each other. The coefficients in the equation can be shown as a ratio:

$$CH_4 : O_2 : CO_2 : H_2O$$
$$1 : 2 : 1 : 2$$

1.3.3 - Apply the state symbols (s), (l), (g) and (aq)

We can balance equations by looking at each type of atom in turn. The balanced equation for the combustion of methane is:

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

We can add symbols to how the physical states of the reactants and products. This is the final step in equation writing. These are:

(g) - gas

(l) - liquid

(s) - solid

(aq) - aqueous (in solution)

These symbols represent the state of each substance at room temperature, unless otherwise specified. Therefore, we would end up with:

$$CH_{4(g)} + 2O_{2(g)} \longrightarrow CO_{2(g)} + 2H_2O_{(g)}$$

All the molecules in this reaction are in the gaseous state.

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:

$$2Mg_{(s)} + O_{2\,(g)} \rightarrow 2MgO_{(s)}$$

We have: 2.431g Mg and excess O_2

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

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

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

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

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. $n = 0.20$ mol
   $m = 4.72g$
   $V = 30\ dm^3$
3. Convert the data for the known quantity to moles, using:
   $n = \frac{m}{M}$ $\quad n = cV$ $\quad n = \frac{N}{L}$ $\quad n = \frac{V}{V_m}$ $\quad n = \frac{PV}{RT}$
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:

$$2C_{(s)} + SiO_{2(s)} \rightarrow SiC_{(s)} + CO_{2(g)}$$

② List relevant data

$m(C) = 40.0\,g$ $\quad M(C) = 12.01\,g\,mol^{-1}$

$m(SiO_2) = 40.0\,g$ $\quad M(SiO_2) = 60.09\,g\,mol^{-1}$

$m(SiC) = x$ $\quad M(SiC) = 40.10\,g\,mol^{-1}$

③ Convert everything into moles

$n(C) = \frac{40.0}{12.01} = 3.331\,mol$ $\qquad n(SiO_2) = \frac{40.0}{60.09} = 0.6657$

④ Determine the excess reagent

$C : SiO_2$
$2 : 1$

$\therefore \frac{1}{2} \times 3.331\,mol\,C = 1.666\,mol\,C \leftarrow$ excess

$\frac{1}{1} \times 0.6657\,mol\,SiO_2 = 0.6657\,mol\,SiO_2$

C is in excess and SiO_2 is the limiting reactant

Find the molar ratio between the LR and unknown quantity

$SiO_2 : SiC$
$1 : 1$

$\therefore n(SiO_2) = n(SiC) = 0.6657\,mol$

⑤ Convert to the relevant units

$n(SiC) = 0.6657 \times 40.10 = 26.69\,g$

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

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

② List given data

$m(N_2) = 42.03g$ $\quad M(N_2) = 28.02 \text{ g mol}^{-1}$

excess H_2

$m(NH_3) = x$ $\quad M(NH_3) = 17.04 \text{ g mol}^{-1}$

③ Convert to moles

$$n(N_2) = \frac{m}{M} = \frac{42.03}{28.02} = 1.500 \text{ mol } N_2$$

④ Find the molar ratio of known and unknown

$N_2 : NH_3$

$1 : 2$

$$n(NH_3) = \frac{2}{1} \times n(N_2) = 3.000 \text{ mol}$$

⑤ Convert to relevant units

$$m(NH_3) = nM = 3.000 \times 17.03 = 51.12g$$

* This is the theoretical yield

⑥ Calculate the percentage yield.

Experimental yield = 45.00g

Theoretical yield = 51.12g

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

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:

$V_1 = 50.0\ dm^3$ $\quad$ $V_2 = x$
$n_1 = 0.00200\ mol$ $\quad$ $n_2 = 0.00375\ mol$

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

$$x = \frac{50.0}{0.00200} \times 0.00375$$

$$= 93.8\ cm^3$$

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:

$$V = \frac{nRT}{P} = \frac{100 \times 8.31 \times 273}{101.3} = 22.4\ dm^3$$

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 dm^3 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:

P_1 and P_2 = the initial and final gas pressures

V_1 and V_2 = the volumes

T_1 and T_2 = the temperatures

n_1 and n_2 = 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:

$P_1 = 760$ mmHg $\qquad P_2 = 180$ mmHg

$V_1 = 95.0\ dm^3 \qquad V_2 = x$

$T_1 = 297$ K $\qquad T_2 = 284$ K

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2} \quad \therefore \quad V_2 = \frac{P_1V_1T_2}{T_1P_2} = \frac{760 \times 95.0 \times 284}{297 \times 180} = 384\ dm^3$$

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

Boyle's Law	$V \propto \frac{1}{P}$	at constant n and T
Charles' Law	$V \propto T$	at constant n and P
Avogadro's Law	$V \propto n$	at constant P and T

$$PV = nRT$$

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 J K^{-1} mol^{-1}

For example:

$$P = 206 \text{ kPa} \qquad V = x$$
$$T = 297 \text{ K} \qquad m = 52.0\text{g}$$
$$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$$

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

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

1.4.8 - Analyse graphs relating to the ideal gas equation

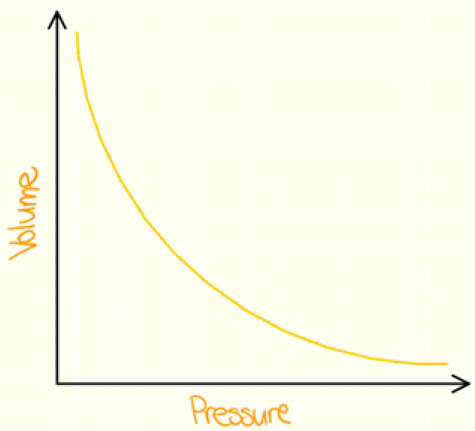
Gas quantities, pressure, volume, amount of gas and temperature are related by a series of mathematical expression known as the gas laws.

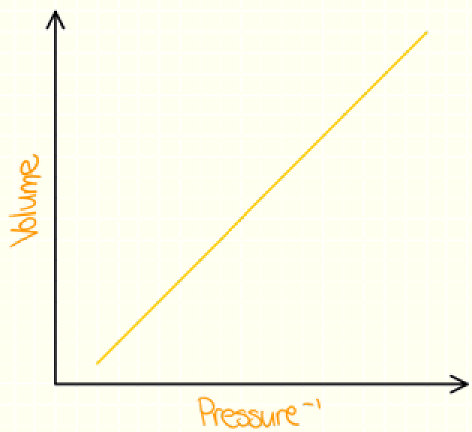
Boyle's Law

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 verses 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:

$P_1 = 750$ mmHg $\qquad P_2 = 620$ mmHg

$V_1 = 1{\cdot}2\text{dm}^3 \qquad V_2 = x$

$$P_1V_1 = P_2V_2 \quad \therefore \quad V_2 = \frac{P_1V_1}{P_2} = \frac{750 \times 1{\cdot}2}{620} = 1{\cdot}5\ \text{dm}^3$$