Topic 1.2

AMOUNT OF SUBSTANCE

The mole
Reacting masses and atom economy
Solutions and titrations
The ideal gas equation
Empirical and molecular formulae
Ionic equations

THE MOLE

Since atoms are so small, any sensible laboratory quantity of substance must contain a huge number of atoms:
1 litre of water contains 3.3×10^{25} molecules.
1 gram of magnesium contains 2.5×10^{22} atoms.
100 cm^3 of oxygen contains 2.5×10^{21}molecules.

Such numbers are not convenient to work with, so it is necessary to find a unit of "amount" which corresponds better to the sort of quantities of substance normally being measured. The unit chosen for this purpose is the **mole**. The number is chosen so that 1 mole of a substance corresponds to its relative atomic/molecular/formula mass measured in grams. A mole is thus defined as follows:

> A mole of a substance is the amount of that substance that contains the same number of elementary particles as there are carbon atoms in 12.00000 grams of carbon-12.

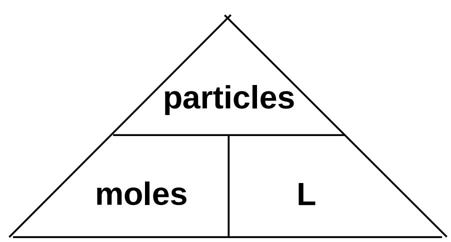
One mole of carbon-12 has a mass of 12.0g.
One mole of hydrogen atoms has a mass of 1.0g.
One mole of hydrogen molecules has a mass of 2.0g.
One mole of sodium chloride has a mass of 58.5g.

The number of particles in one mole of a substance is 6.02×10^{23}. This is known as **Avogadro's number, L**.

Thus when we need to know the number of particles of a substance, we usually count the number of moles. It is much easier than counting the number of particles.

The number of particles can be calculated by multiplying the number of moles by Avogadro's number. The number of moles can be calculated by dividing the number of particles by Avogadro's number.

(Number of particles) = (number of moles) x L



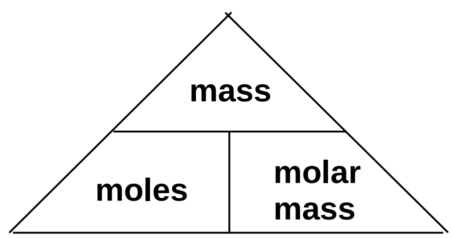
The mass of one mole of a substance is known as its **molar mass**, and has units of $gmol^{-1}$. It must be distinguished from relative atomic/molecular/formula mass, which is a ratio and hence has no units, although both have the same numerical value.

The symbol for molar mass of compounds or molecular elements is m_r. The symbol for molar mass of atoms is a_r.

Mass (m), molar mass (m_r or a_r) and number of moles (n) are thus related by the following equation:

MASS = MOLAR MASS X NUMBER OF MOLES
or $m = m_r \times n$

Mass must be measured in grams and molar mass in $gmol^{-1}$.



REACTING MASSES

It is possible to use the relationship moles = mass/m_r to deduce the masses of reactants and products that will react with each other.

When performing calculations involving reacting masses, there are two main points which must be taken into account:

The total combined mass of the reactants must be the same as the total combined mass of the products. This is known as the law of conservation of mass.

The ratio in which species react corresponds to the number of moles, and not their mass. Masses must therefore all be converted into moles, then compared to each other, then converted back.

i) reactions which go to completion

Eg What mass of aluminium will be needed to react with 10 g of CuO, and what mass of Al_2O_3 will be produced?

$3CuO(s) + 2Al(s) \rightarrow Al_2O_3(s) + 3Cu(s)$
10 g
= 10/79.5
= 0.126 moles of CuO
3:2 ratio with Al
so 2/3 x 0.126 = 0.0839 moles of Al, so mass of Al = 0.0839 x 27 = 2.3 g
3:1 ratio with Al_2O_3
so 1/3 x 0.126 = 0.0419 moles of Al_2O_3, so mass of Al_2O_3 = 0.0419 x 102 = 4.3 g

ii) reactions which do not go to completion

Many inorganic reactions go to completion. Reactions which go to completion are said to be **quantitative**. It is because the reactions go to completion that the substances can be analysed in this way.

Some reactions, however, particularly organic reactions, do not go to completion. It is possible to calculate the **percentage yield** of product by using the following equation:

$$\% \text{ yield} = \frac{\text{amount of product formed}}{\text{maximum amount of product possible}} \times 100$$

Eg 2.0 g of ethanol (C_2H_5OH) is oxidised to ethanoic acid (CH_3COOH). 1.9 g of ethanoic acid is produced. What is the percentage yield? (assume 1:1 ratio)

Moles of ethanol = 2/46 = 0.0435
Max moles of ethanoic acid = 0.0435
so max mass of ethanoic acid = 0.0435 x 60 = 2.61 g
percentage yield = 1.9/2.61 x 100 = 73%

Eg When propanone (CH_3COCH_3) is reduced to propan-2-ol ($CH_3CH_2CH_2OH$), a 76% yield is obtained. How much propan-2-ol can be obtained from1.4 g of propanone? (assume 1:1 ratio)

Moles of propanone = 1.4/58 = 0.0241 moles
So max moles of propan-2-ol produced = 0.0241 moles
So actual amount produced = 0.0241 x 76/100 = 0.0183 moles
So mass of propan-2-ol = 0.0183 x 60 = 1.1 g

ATOM ECONOMY

When we carry out a chemical reaction in order to make a product, we often make other products, called by-products, as well.

Eg In the production of NaOH from NaCl the following reaction takes place:

$$2NaCl + 2H_2O \rightarrow 2NaOH + H_2 + Cl_2$$

The atom economy of a reaction is the percentage of the total mass of reactants that can, in theory, be converted into the desired product. It can be calculated as follows:

$$\boxed{\textbf{\% atom economy} = \frac{\textbf{mass of desired product}}{\textbf{total mass of products}} \times \textbf{100}}$$

Assuming we start with 2 moles of NaCl and 2 moles of H_2O, we will make 2 moles of NaOH, and 1 mole of H_2 and Cl_2.

$$\text{So \% atom economy} = \frac{(2 \times 40)}{(2 \times 40) + (1 \times 2) + (1 \times 71)} \times 100 = 52.3\ \%$$

The remaining 47.7% of the mass is converted into less useful products and is hence wasted.

So the higher the atom economy, the less waste and the more efficient the product process (assuming the reaction does actually go to completion).

All reactions which have only one product have an atom economy of 100%

Atom economy is an important consideration when considering how to make a particular useful product.

SOLUTIONS

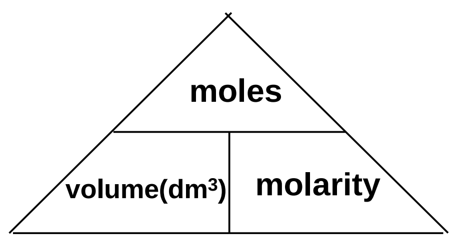
A **solution** is a homogeneous mixture of two or more substances in which the proportions of the substances are identical throughout the mixture.

The major component of a solution is called the **solvent** and the minor components are called the **solutes**. In most cases water is the solvent.

The amount of solute present in a fixed quantity of solvent or solution is called the **concentration** of the solution. It is usually measured in grams of solute per dm^3 of solution or in moles of solute per dm^3 of solution. In the latter case ($moldm^{-3}$) it is also known as the **molarity** of the solution.

The number of moles of solute, molarity of the solution and volume of solution can thus be related by the equation:

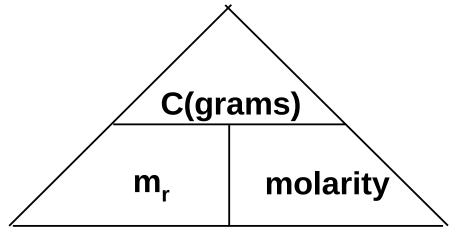
$$\textbf{Number of moles = volume x molarity}$$
$$\mathbf{n = C \times V}$$



The volume of solution in this case must always be measured in dm^3 (or litres). If the volumes are given in cm^3 then V/1000 must be used instead.

If concentration is given in gdm^{-3}, it must be converted to molarity before it can be used in the above equation. This can be done easily by dividing by the molar mass of the solute.

$$\textbf{Concentration } (\mathbf{gdm^{-3}}) \textbf{ = Molarity x molar mass}$$
$$\textbf{Or } \mathbf{C_g = C_m \times m_r}$$



The volume of one solution required to react with a known volume of another can be deduced from the above relationships and knowledge of the relevant chemical equation. Remember it is moles which react in the ratio shown, so all quantities must be converted to moles before the comparison can be made.

The quantitative investigation of chemical reactions by comparing reacting volumes is known as **volumetric analysis**. The procedure by which reacting volumes are determined is known as a **titration**.

In titrations, a solution whose concentration is unknown is titrated against a solution whose concentration is known. The solution of known concentration is always placed in the burette, and the solution of unknown concentration is always placed in the conical flask.

Eg 28.3 cm^3 of a 0.10 $moldm^{-3}$ solution of NaOH was required to react with 25 cm^3 of a solution of H_2SO_4. What was the concentration of the H_2SO_4 solution?
Equation: $H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$

Moles of NaOH = 28.3/1000 x 0.1 = 2.8 x 10^{-3}
2:1 ratio so moles of H_2SO_4 = 2.8 x 10^{-3}/2 = 1.4 x 10^{-3}
so concentration of H_2SO_4 = 1.4 x 10^{-3}/25 x 1000 = 0.056 $moldm^{-3}$.

Eg Calculate the volume of 0.50 $moldm^{-3}$ nitric acid required to react completely with 5 g of lead (II) carbonate.
Equation: $PbCO_3 + 2HNO_3 \rightarrow Pb(NO_3)_2 + CO_2 + H_2O$

Moles of $PbCO_3$ = 5/267 = 0.0187
1:2 ratio so moles of HNO_3 = 0.0187 x 2 = 0.0375
Volume of HNO_3 = 0.0375/0.5 x 1000 = 74.9 cm^3.

GASES

The volume occupied by a gas depends on a number of factors:

i) **the temperature**: the hotter the gas, the faster the particles are moving and the more space they will occupy
ii) **the pressure**: the higher the pressure, the more compressed the gas will be and the less space it will occupy
iii) **the amount of gas**: the more gas particles there are, the more space they will occupy

The volume occupied by a gas does not depend on what gas it is, however: one mole of any gas, at the same temperature and pressure, will have the same volume as one mole of any other gas.

The pressure, temperature, volume and amount of gas can be related by a simple equation known as the **ideal gas equation**:

$$\boxed{\mathbf{PV = nRT}}$$

P is the pressure measured in pascals (Pa) or Nm^{-2}. One atmosphere, which is normal atmospheric pressure, is 101325 Pa.

V is the volume in m^3. Remember; $1\ m^3 = 1000\ dm^3 = 10^6\ cm^3$.

T is the absolute temperature, measured in Kelvin (K). Remember; $0\ ^oC = 273\ K$.

R is the molar gas constant and has a value of 8.31 $Jmol^{-1}K^{-1}$.

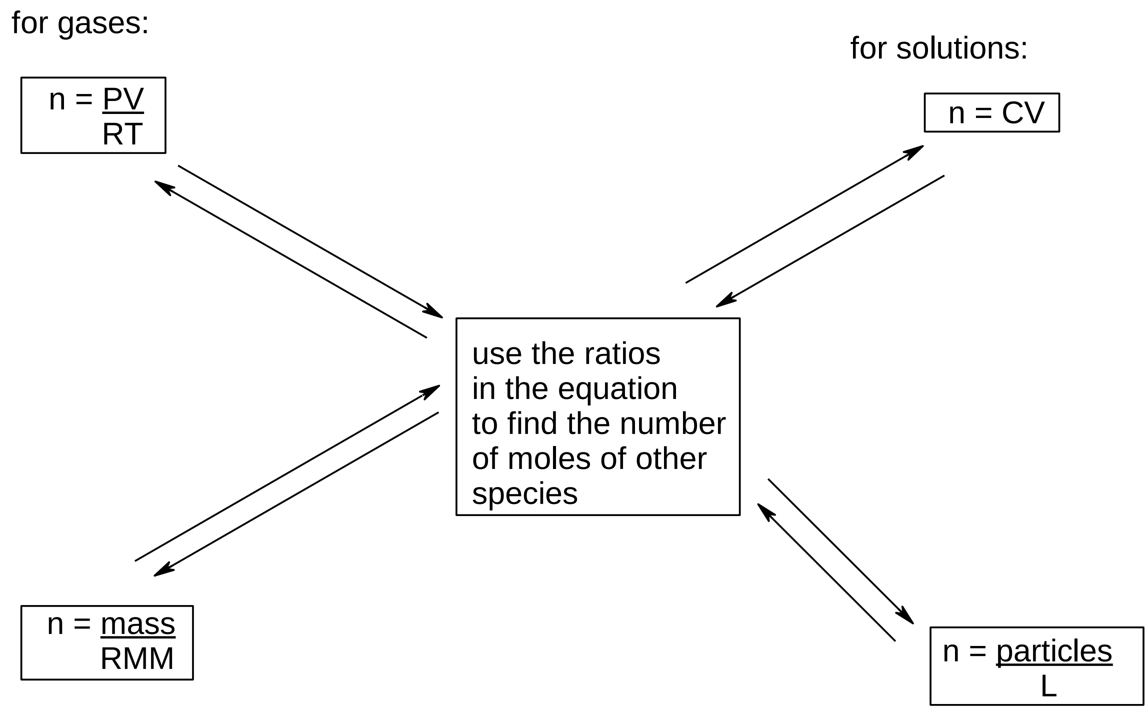
This equation can be rearranged to find the density of gases and the RMM of gases, using the relationship $m = n \times m_r$.

$PV = mRT/m_r$, so the mass of one mole is given by $m_r = mRT/PV$, where m is the mass in kg. The answer m will also be in kg so it must be converted into grams.

The density of a gas, or mass/volume, is given by $(m/V) = m_rP/RT$.

SUMMARY – USING MOLES

Using the four relationships described, it is possible to calculate the amount of any substance in a chemical reaction provided that the chemical equation is known and the amount of one of the reacting species is also known. The procedure is summarised in the table below:



These relationships are frequently used in practical chemistry. Typical calculations in AS Practical Chemistry involve:

i) Determining the concentration of a solution

ii) Determining the relative molecular mass of a solid

iii) Determining the percentage purity of a solid

The percentage purity of a substance can be calculated as follows:

$$\text{Percentage purity} = \frac{\text{mass substance would have if it was pure}}{\text{mass of impure substance}} \times 100$$

EMPIRICAL AND MOLECULAR FORMULAE

The **empirical formula** of a compound is the formula which shows the simplest whole-number ratio in which the atoms in that compound exist.
It can be calculated if the composition by mass of the compound is known.

The **molecular formula** of a substance is the formula which shows the number of each type of atom in the one molecule of that substance.
It applies only to molecular substances, and can be deduced if the empirical formula and molar mass of the compound are known.

The molecular formula is always a simple whole number multiple of the empirical formula.

Eg a substance contains 85.8% carbon and 14.2% hydrogen, what is its empirical formula? If its relative molecular mass is 56, what is its molecular formula?

Mole ratio = $\frac{85.8}{12} : \frac{14.2}{1}$

$= \frac{7.15}{7.15} : \frac{14.2}{7.15}$

$= 1 : 2$ so empirical formula = CH_2

RMM = 56 = (CH_2) so 14n = 56 and n = 56/14 = 4

Molecular formula = C_4H_8

It is also possible to calculate the percentage composition by mass of a substance, if its empirical or molecular formula is known.

Eg What is the percentage composition by mass of ethanoic acid, $C_2H_4O_2$?

RMM = 60

% C = (12 x 2)/60 x 100 = 40.0%

% H = (1 x 4)/60 x 100 = 6.67%

%O = (16 x 2)/60 x 100 = 53.3%

FORMULAE OF IONIC COMPOUNDS

An ion is a species in which the number of electrons is not equal to the number of protons. An ion thus has an overall charge, characteristic of the difference in the number of protons and electrons. Ions with a positive charge are known as **cations** and ions with a negative charge are known as **anions**.

Compounds made up of ions are known as **salts**. They are all electrically neutral, so must all contain at least one anion and at least one cation.

Salts do not have molecular formulae, as they do not form molecules. They are written as unit formulae.

The **unit formula** of an ionic compound is the formula which shows the simplest whole number ratio in which the ions in the compound exist. This depends on the charges of the ions involved. Some important ions and their charges are shown below:

i) cations

Charge	Formula	Name
+1	Na^+	Sodium
+1	K^+	Potassium
+1	Ag^+	Silver
+1	H^+	Hydrogen
+1	NH_4^+	Ammonium
+1	Cu^+	Copper(I)
+2	Mg^{2+}	Magnesium
+2	Ca^{2+}	Calcium
+2	Fe^{2+}	Iron(II)
+2	Zn^{2+}	Zinc
+2	Pb^{2+}	Lead(II)
+2	Cu^{2+}	Copper(II)
+2	Ni^{2+}	Nickel(II)
+3	Al^{3+}	Aluminium
+3	Cr^{3+}	Chromium(III)
+3	Fe^{3+}	Iron(III)

Note that some atoms can form more than one stable cation. In such cases it is necessary to specify the charge that is on the cation by writing the charge in brackets after the name of the metal.

ii) anions

Charge	Formula	Name
-1	OH^-	Hydroxide
-2	SO_4^{2-}	Sulphate
-2	CO_3^{2-}	Carbonate
-1	NO_3^-	Nitrate
-1	HCO_3^-	Hydrogencarbonate

CHEMICAL EQUATIONS

The purpose of chemistry is essentially to study chemical reactions. In chemical reactions, elements or compounds react with each other to form other elements and/or other compounds.

Chemical reactions involve the movement of electrons between different species. The nuclei always remain intact.

Every chemical reaction can be represented by a chemical equation. A chemical equation indicates the species involved in the reaction and shows the way in which they react. Every chemical equation must contain three pieces of information:

i) the identities of all the reactants and products

The chemical formulae of all the species involved in the reaction should be shown. Any species left unchanged should be left out. Reactants must be written on the left of the arrow and products on the right.

Remember that in chemical reactions all the nuclei remain unchanged. Therefore the total number of atoms of each type must be the same on each side of the equation. Atoms themselves cannot be created or destroyed in chemical reactions; only transferred from species to species.

ii) the reaction coefficients

Atoms, elements and compounds combine with each other in simple whole number ratios, eg 1:1, 1:2, 1:3. The ratio in which the species react and in which products are formed are shown in the reaction coefficients. These are the numbers which precede the chemical formula of each species in the equation. If no coefficient is shown it is assumed to be 1.

Deducing the reaction coefficients for a reaction is known as balancing the equation. The total number of atoms of each element must be the same on both sides of the equation.

When balancing chemical equations, always balance compounds first and elements second. It's easier that way.

N.B. Reaction coefficients in no way show the actual amount of a substance which is reacting. They provide information only on the way in which they react.

iii) The state symbols

The state symbol shows the physical state of each reacting species and must be included in every chemical equation. There are four state symbols required for A-level chemistry:
(s) - solid
(l) - liquid
(g) - gas
(aq) - aqueous, or dissolved in water

IONIC EQUATIONS

Many reactions that take place in aqueous solution do not involve all of the ions that are written in the equation. Some species remain in aqueous solution before and after the reaction. They therefore play no part in the reaction and are known as **spectator ions**.

In **ionic equations**, spectator ions are left out.

Eg $BaCl_2(aq) + Na_2SO_4(aq) \rightarrow BaSO_4(s) + 2NaCl(aq)$
This reaction involves the precipitation of barium sulphate.
Notice that the Cl^- ions and the Na^+ ions remain in the aqueous state before and after the reaction. They are therefore spectator ions.
The above reaction can then be rewritten as follows:
$Ba^{2+}(aq) + SO_4^{2-}(aq) \rightarrow BaSO_4(s)$

Eg $Al_2(SO_4)_3(aq) + 6NaOH(aq) \rightarrow 2Al(OH)_3(s) + 3Na_2SO_4(aq)$
This reaction involves the precipitation of aluminium hydroxide.
The Na^+ and SO_4^{2-} ions are spectator ions and can be left out
The ionic equation for the reaction is:
$Al^{3+}(aq) + 3OH^-(aq) \rightarrow Al(OH)_3(s)$

Ionic equations are very useful for simplifying **precipitation** reactions.

They can also simplify **acid-base** reactions:

Eg $NaOH(aq) + HCl(aq) \rightarrow NaCl(aq) + H_2O(l)$
The Na^+ and Cl^- ions are spectator ions, so the ionic equation for the reaction is:

$$\mathbf{H^+(aq) + OH^-(aq) \rightarrow H_2O(l)}$$

All reactions between strong acids and strong alkalis have the same ionic equation.