FORMULAE, EQUATIONS AND MOLES

Important terms
In order to use formulae and equations it is necessary to understand the meaning of important terms.

Atom	The smallest unit of an element that can exist
Molecule	The smallest part of an element or a compound which can exist alone under normal conditions.
Ion	An atom or group of atoms possessing a negative charge
Element	A substance containing just one type of atom.
Compound	A substance that contains different elements that have been chemically combined
Empirical formulae	The simplest ratio showing the different types of atom present in a substance.
Molecular formulae	The actual numbers of each type of atom in a molecule of the substance.

Amount of Substance

Avagadro's Constant and the Mole
In order to carry out quantitative investigations in chemistry it is necessary to be able to 'count' atoms. This is done using the mole. A mole contains a given number (the Avogadro constant) of atoms or other particles, and this is measured by mass.

If we take a mole of atoms of a particular element, the mass will be the Relative Atomic Mass for that element.

The Avogadro constant is the number of particles in 1 mole of substance (6.023×10^{23})

The **mole** is the amount of a substance that contains the same number of particles as there are atoms in 12.00g of carbon-12. This number of atoms is 6.02×10^{23} and is called the **Avogadro constant**.

$$\text{Amount of substance} = \frac{\text{number of particles}}{\text{Avogadro constant}}$$

Moles from mass

To find the number of moles of atoms we use the formula:

$$\text{Moles} = \frac{\text{mass of substance}}{\text{relative atomic mass}}$$

If we take a mole of ionic lattice or molecules of a material, the mass will be the molar mass

To find the number of moles of molecules or compounds we can use the formula:

$$\text{Moles} = \frac{\text{mass}}{\text{molar mass (RFM, } M_r\text{)}}$$

Examples

1. Calculate the number of moles in 10g magnesium sulphate ($MgSO_4$.)

   Molar mass of $MgSO_4$ = 24 + 32 + (4x 16) = 120

   Moles = 10 /120 = <u>0.083 mol</u>

2. Calculate the mass of 0.04mol Copper(II)nitrate

   Molar mass of $Cu(NO_3)_2$ = 63.5 + (2 x 14) + (6x 16) = 178.5

   Mass = Moles x Formula mass

   = 0.04 x 178.5 = <u>7.5g</u>

Formulae determination

An **empirical formula** is the simplest formula which shows the ratio of each type of atom present in a compound.
A **molecular formula** is a simple multiple of the empirical formula showing how many of each type of atom are present in a compound.

The formula of a compound can be calculated from the mass of elements in it. This is done as follows:

Step 1: From the mass of each element find the number of moles.
Step 2: From the number of moles find the simplest ratio.
Step 3: Convert the mole ratio to a whole number ratio; this gives the formula.

Example
A hydrocarbon consists of 14.4g carbon and 1.2g hydrogen. Calculate its empirical formula.

	C		H
	14.4 / 12		1.2 / 1
	=1.2 mol		=1.2 mol
Ratio =	1	:	1

So the empirical formula is CH

If we try to work out the structure of this we can see that this is not the formula of the molecule. To find this formula we need to know the molecular mass.

If the molar mass of this compound is 78gmol^{-1}, what is the molecular formula?

CH has a mass of 13
the number of these units is 78/13 = 6
so the formula is C_6H_6

A similar process is used to find formulae from percentage composition.

Example
A carbohydrate is composed of 40.00% Carbon, 6.67% Hydrogen and 53.33% Oxygen.
It has a molar mass of 120gmol^{-1}. Calculate the molecular formula.

	C		H		O
	40.00 / 12		6.67 / 1		53.33 / 16
	= 3.33		= 6.67		= 3.33
Ratio	1	:	2	:	1

Empirical formula : CH_2O
mass : *30*
so number of units = 120 / 30 = 4
Molecular formula = $C_4H_8O_4$

Moles of gas

One mole of any gas has approximately the same volume as any other gas at a particular temperature and pressure. (This is **Avogadro's Law**).

Example: $2\ C_4H_{10} + 13\ O_2 \rightarrow 8\ CO_2 + 10\ H_2O$

What volume of oxygen is needed to react with 15 cm^3 of butane under room conditions?

> *From the equation, 1 mole of butane reacts with 6.5 moles of oxygen.*
> *Therefore, 1 volume of butane needs 6.5 volumes oxygen.*
> *Therefore, 15 cm^3 of butane needs $15 \times 6.5 = 97.5$ cm^3 oxygen.*

At room temperature and 1Atm this is 24dm^3 (24000cm^3). (At 0^{o}C and 1Atm this is 22.4dm^3).

So the number of moles of a gas at room temperature can be found from the formula.

$$\boxed{\text{Moles} = \frac{\text{Volume (in dm}^3)}{24}}$$

Example. *Calculate the moles of carbon dioxide in 480cm^3 of the gas.*

Moles = 480 / 24,000 = 0.002

Moles in solution

The concentration of solutions is also expressed in terms of moles.

$$\boxed{\text{Concentration} = \frac{\text{Moles}}{\text{Volume (in dm}^3)}}$$

The concentration of a solution can be stated as the mass of solute per cubic decimeter of solution (g/dm^3) or the amount in moles of a solute present in 1dm^3 of solution (mol/dm^3).

To make a solution of 1mol dm^{-3} concentration, 1mol of substance is dissolved and the solution made up to a total volume of 1dm^3.

Examples

1. Calculate the concentration of a solution containing 2.4g $MgSO_4$ in 500cm^3 of solution.

Moles = 2.4 / 120 = 0.02mol
Concentration = 0.02mol / 0.5dm^3 = 0.04moldm^{-3}

2. Calculate the mass of NaOH required to make 100cm^3 of a 0.2 mol dm^{-3} solution.

Moles = Concentration x Volume (dm^3)
= 0.2 x 0.1 = 0.02mol

Mass = Moles x Formula mass
= 0.02 x 40 = 0.8g

Parts per million

This is a way of expressing very dilute concentrations of substances (usually pollutants).
Just as per cent means out of a hundred, so parts per million or ppm means out of a million.

Usually describes the concentration of something in water or soil.
One ppm is equivalent to **1 milligram per dm^3 of water (mg/dm^3)**
or 1 milligram per kilogram soil (mg/kg).

or the volume of a gas pollutant in air.
One ppm is equivalent to **1 cm^3 per 1 000 dm^3 of air (1 000 000 cm^3)**

Example
A 250 cm^3 sample of river water was found to contain 56 ppm of gold.
Calculate the mass of gold in the 250cm^3 sample of river water.

The sample contains 56 ppm of gold = 56 mg per dm^3 of river water = 56 mg per 1000cm^3

1 cm^3 of water contains 56 / 1000 mg = 0.056 mg of gold
25 cm^3 of water contains 0.056 x 25 = 1.4 mg = 1.4 x 10^{-3} g of gold

Example
Chronic exposure to CO at concentrations of 70 ppm or greater causes cardiac damage.
Would you be at serious risk if you were exposed 380 cm^3 of carbon monoxide in a 3500 dm^3 room?

380 cm^3 in 3500000 cm^3 = 380 cm^3 in 3.5 million cm^3 = 380 / 3.5 = ***108.6 ppm – You are at risk!***

<u>Reacting quantities and chemical equations</u>

<u>Chemical equations and mass calculations</u>
Mole calculations can be used together with chemical equations to determine the quantity of material formed or used up in a chemical reaction.
Whether using masses, volumes of solutions (of known concentration), or volumes of gases the same general method can be used.

Step 1: Find the number of moles of one substance
Step 2: Use the mole ratio from the chemical equation to find how many moles of the other substance will be formed / used up.
Step 3: From the number of moles of this substance calculate the mass / volume / concentration of the desired substance.

Example 1:
Calculate the mass of Iron(II)sulphate ($FeSO_4$), which can be produced from 7.84g of H_2SO_4.

$$Fe + H_2SO_4 \rightarrow FeSO_4 + H_2$$

Step 1 - *Moles of H_2SO_4 used = mass / RFM = 7.84 / 98 = 0.08*
Step 2 - *From equation 1 mol H_2SO_4 forms 1mol of Iron(II)sulphate*
So mole of Iron(II)sulphate = 0.08
Step 3 – *Mass of Iron(II)sulphate = moles x RFM = 0.08 x 152 = 12.2g (3 sig.fig.)*

Example 2:
What mass of aluminium is needed to react with 7.00g of anhydrous $CuSO_4$?

$$2Al + 3CuSO_4 \rightarrow Al_2(SO_4)_3 + 3Cu$$

Step 1 - *Moles of $CuSO_4$ used = mass / RFM = 7 / 159.5 = 0.0439 mol*
Step 2 - *From equation, 3 mol of $CuSO_4$ react with 2 mol of Al.*
So 1 mol of $CuSO_4$ reacts with ⅔ mol of Al.
So 0.0439 mol $CuSO_4$ reacts with $0.0439 \times \frac{2}{3}$ = 0.0293 mol Al

Step 3 – *Mass of Al = moles x RFM = 0.0239 mol $\times$ 27 g/mol = <u>0.790 g</u> (3 sig.fig.)*

Example 3:
Calculate the volume carbon dioxide gas which will be produced from the combustion of 2.20g of propane (C_3H_8).

$$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$$

Step 1 - *Moles of propane used = mass / RFM = 2.20 / 44 = 0.05 mol*
Step 2 - *From equation 1mol propane forms 3mol carbon dioxide*
So mole of carbon dioxide = 0.15 mol
Step 3 - *Volume of carbon dioxide = moles x 24000 = 0.15 x 24,000 = 3,600cm^3*

Titrations

A titration is a method of finding out how much of one material will react with how much of another.

Carrying out the titration

1. A pipette-filler is added to the volumetric pipette.
2. Some of the solution is drawn into the pipette. The pipette is tilted and rotated so that all the surfaces are rinsed in the solution.
3. The rinsing solution is then discarded.
4. The solution is drawn into the pipette until the bottom of the meniscus is on the mark.
5. The solution is then released into a clean conical flask.
6. When no more solution emerges from the burette, touch the tip of the pipette against the side of the conical flask. Some of the liquid will remain in the tip and this should be left as the pipette is calibrated to allow for this.
7. A suitable indicator should be added to the conical flask
8. The flask is placed on a white tile under a burette.
9. The flask should be held in the right hand (or writing hand) and swirled.
10. The burette tap should be controlled by the left hand, first and second fingers behind the tap and the thumb in front of it. Add the solution from the burette until the indicator changes colour. Note the reading on the burette. This is the rough reading.
11. Discard the contents of the flask and rinse it with tap water and then distilled water.
12. Repeat the process, adding the solution from the burette fairly slowly with continual stirring. As the level in the burette approaches that of the rough reading, the solution is added drop by drop. When one drop changes the colour of the indicator, allow the solution to drain down the sides of the burette before taking the reading.
13. Accurate burette readings should be recorded to two decimal places, the second decimal place being 0 or 5.
14. Readings should continue to be taken in this way until one rough and two accurate readings that are within 0.1 cm^3 of each other – concordant readings - are obtained.
15. Calculations should be based on the mean average of the two concordant readings.

Titration calculations

Use the same three step method as before.

Example

If 23.45 cm^3 of 0.2 mol dm^{-3} sodium hydroxide react with 25.0cm^3 of sulphuric acid. Find the concentration of the acid.

$$2NaOH + H_2SO_4 \rightarrow Na_2SO_4 + 2H_2O$$

Step 1 - *Moles of NaOH = 23.45 / 1000 x 0.2 = 0.00469 mol*

Step 2 - *Moles of H_2SO_4 = 0.00469 / 2 = 0.002345 mol*

Step 3 - *Concentration of H_2SO_4 = 0.002345 / 0.025 = 0.0938 mol dm^{-3} (3 sig.fig.)*

Percentage Yield

Chemical reactions are carried out in the laboratory and by industry to make new materials. In the process of producing new substances, some material is lost.
The efficiency of the conversion process is measured using percentage yield or atom economy.

$$\% \text{ Yield} = \frac{\text{Actual Mass of material produced}}{\text{Theoretical maximum mass which could be produced}} \times 100$$

Example

In the preparation of copper sulphate, a solution of sulphuric acid containing 2.00g of the pure acid, is reacted with an excess of copper oxide.
4.37g of the hydrated copper sulphate, $CuSO_4.5H_2O$ was produced. Calculate the % yield.

$$CuO + H_2SO_4 \rightarrow CuSO_4 + H_2O$$

Moles of sulphuric acid used =mass / RFM = 2.00 / 98 = 0.05 = 0.0204mol

From equation 1mol sulphuric acid forms 1mol copper sulphate
So moles of copper sulphate formed = 0.0204mol

Molar mass of hydrated copper sulphate = 63.5 + 32 + 64 + 90 = 249.5
Theoretical maximum mass which could be produced = 249.5 x 0.0204 = 5.09g

*% Yield = Actual yield / theoretical x 100 = 4.37 / 5.09 x 100 = **85.9%***

Atom Economy

Whereas the percentage yield gives us information about the actual efficiency of a reaction, atom economy examines the theoretical potential yield of a reaction, by considering the quantity of starting atoms in all the reactants end up in the desired product.

$$\% \text{ atom economy} = \frac{\text{Molar mass of useful product}}{\text{Total molar mass of starting materials}} \times 100$$

Taking the laboratory preparation of copper(II) sulphate from sulphuric acid and copper(II) oxide as an example.

$$CuO + H_2SO_4 \rightarrow CuSO_4 + H_2O$$

Mass of starting atoms is	Mass of desired product is
CuO = 63.5 + 16 = 79.5	$CuSO_4$ = 63.5 + 32 + 64 = 159.5
H_2SO_4 = 2 + 32 + 64 = 98	
Total = 177.5	

$$\% \text{ atom economy} = \frac{159.5}{177.5} \times 100 = 89.9\%$$

The atom economy for the production of ethanol from ethene and steam is shown below.

$$C_2H_4 + H_2O \rightarrow C_2H_5OH$$

% atom economy = 46 / 46 x 100 = 100% (there are no unwanted products).

Derivation of Equations

An equation can be derived or confirmed by measuring quantities of substances involved in the reaction.

Equations can be written to explain simple test tube reactions such as displacement and precipitation.

Example 1

1.74g of manganese(IV) oxide is added to an excess of concentrated hydrochloric acid and warmed. The chlorine given off was absorbed and weighed. The mass of chlorine given off was 1.42g. Another product of the reaction was purified and analysed.
It was found that this salt contained 1.10g of manganese and 1.42g of chlorine.
(a) Determine the formula of the salt.
(b) Calculate the number of moles of manganese(IV) oxide used in the reaction.
(c) Calculate the number of moles of chlorine and salt produced in the reaction.
(d) Write a chemical equation for the reaction.

(a)	*Mn*		*Cl*	
	1.10 / 55		*1.42 / 35.5*	
	=0.02 mol		*=0.04 mol*	
Ratio =	*1*	*:*	*2*	*Formula = $MnCl_2$*

(b) Moles MnO_2 = mass / RFM = 1.74 / 87 = 0.02 mol

(c) Moles Cl_2 produced = mass / RFM = 1.42 / 71 = 0.02 mol
Moles $MnCl_2$ produced = mass / RFM = 2.52 / 126 = 0.02 mol

Equation:	MnO_2 + HCl	→	$MnCl_2$	+ Cl_2	+ ?
Moles	0.02		0.02	0.02	
Mole ratio	1		1	1	

Balancing for Cl: $MnO_2 + 4HCl \rightarrow MnCl_2 + Cl_2 + ?$
Balancing for H & O: $MnO_2 + 4HCl \rightarrow MnCl_2 + Cl_2 + 2H_2O$

Example 2

For the following reactions, write chemical and ionic equations using state signs.

(a) When dilute nitric acid is added to sodium carbonate solution, effervescence occurs and the gas formed turns limewater cloudy.

$$Na_2CO_{3(aq)} + 2HNO_{3(aq)} \rightarrow 2NaNO_{3(aq)} + H_2O_{(l)} + CO_{2(g)}$$
$$CO_3^{2-}{}_{(aq)} + 2H^+{}_{(aq)} \rightarrow H_2O_{(l)} + CO_{2(g)}$$

(b) When iron filings are added to copper sulphate solution, the blue solution turns green and the grey solid is replaced by a red-brown solid.

$$CuSO_{4(aq)} + Fe_{(s)} \rightarrow FeSO_{4(aq)} + Cu_{(s)}$$
$$Cu^{2+}{}_{(aq)} + Fe_{(s)} \rightarrow Fe^{2+}{}_{(aq)} + Cu_{(s)}$$

(c) When silver nitrate solution is added to sodium chromate solution, a red ppt forms.

$$Na_2CrO_{4(aq)} + 2AgNO_{3(aq)} \rightarrow 2NaNO_{3(aq)} + Ag_2CrO_{4(s)}$$
$$CrO_4^{2-}{}_{(aq)} + 2Ag^+ \rightarrow Ag_2CrO_{4(s)}$$