1 Atoms, molecules and stoichiometry

DEFINITION: **Relative atomic mass (*Ar*)** is the **average mass** of one atom compared to one twelfth of the mass of one atom of carbon-12

DEFINITION: **Relative Isotopic mass** is the **mass** of one isotope compared to one twelfth of the mass of one atom of carbon-12

DEFINITION: **Relative molecular mass (*Mr*)** is the weighted **average mass** of a molecule compared to one twelfth of the mass of one atom of carbon-12

DEFINITION: **Relative formula mass (*Mr*)** is the weighted **average masses** of the **formula** units compared to one twelfth of the mass of one atom of carbon-12

The term molecule should only be used for covalent molecules. For ionic substances use the term relative formula mass. They are, however, calculated in the same way.

The mole

The mole is the key concept for chemical calculations

DEFINITION: **The mole** is the amount of substance in grams that has the same number of particles as there are atoms in 12 grams of carbon-12.

Avogadro's Number

There are 6.022 x 10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.022 x 10^{23} of that entity':

For pure solids, liquids and gases

$$\text{moles} = \frac{\text{mass}}{Mr}$$

Unit of Mass: grams
Unit of moles : mol

Relative Formula mass (*M*r) for a compound can be calculated by adding up the relative atomic masses(from the periodic table) of each element in the compound
eg $CaCO_3$ = 40.1 + 12.0 +16.0 x3 = 100.1

Many questions will involve changes of units
1000 mg =1g
1000 g =1kg
1000kg = 1 tonne

Example 1: What is the number of moles in 35.0g of $CuSO_4$?

moles = mass/*M*r

= 35.0/ (63.5 + 32.0 +16.0 x4)

= 0.219 mol

Example 2: What is the number of moles in 75.0mg of $CaSO_4.2H_2O$?

moles = mass/*M*r

= 0.075/ (40 + 32.0 +16.0 x4 + 18.0x2)

= 4.36x10^{-4} mol

Avogadro's Constant can be used for atoms, molecules and ions

1 mole of copper atoms will contain 6.022 x 10^{23} atoms
1 mole of carbon dioxide molecules will contain 6.022 x 10^{23} molecules
1 mole of sodium ions will contain 6.022 x 10^{23} ions

No of particles = moles of substance (in mol) X Avogadro's constant (L)

Example 3 : How many atoms of Tin are there in a 6.00 g sample of Tin metal?

moles = mass/*Ar*

= 6.00/ 118.7

= 0.05055 mol

Number atoms = moles x 6.022 x 10^{23}

= 0.05055 x 6.022 x 10^{23}

= 3.04 x10^{22}

Example 4 : How many chloride ions are there in a 25.0 cm^3 of a solution of magnesium chloride of concentration 0.400 $moldm^{-3}$?

moles= concentration x Volume

$MgCl_2$= 0.400 x **0.0250**

= 0.0100 mol

moles of chloride ions = 0.0100 x2

= 0.0200

There are two moles of chloride ions for every one mole of $MgCl_2$

Number ions of Cl^- = moles x 6.022 x 10^{23}

= 0.0200 x 6.022 x 10^{23}

= 1.20 x10^{22} (to 3 sig fig)

Determination of Relative Atomic Mass

The relative atomic mass quoted on the periodic table is a weighted average of all the isotopes

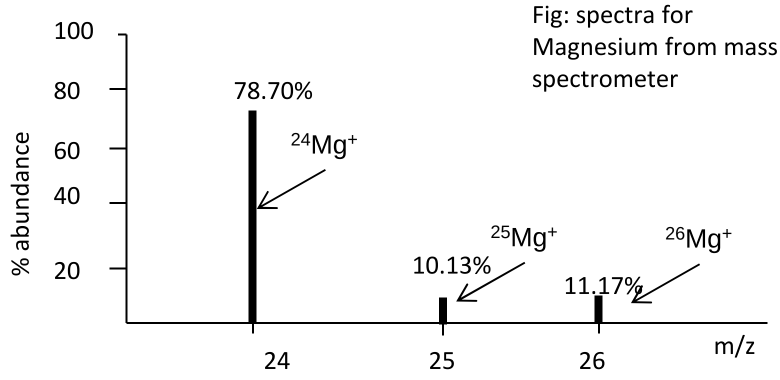


Fig: spectra for Magnesium from mass spectrometer

If asked to give the species for a peak in a mass spectrum then give charge and mass number e.g. $^{24}Mg^{+}$

$$\text{R.A.M} = \frac{\Sigma\ (\text{isotopic mass x \% abundance})}{100}$$

Use these equations to work out the R.A.M

For above example of Mg
R.A.M = [(78.7 x 24) + (10.13 x 25) + (11.17 x 26)] /100 = 24.3

$$\text{R.A.M} = \frac{\Sigma\ (\text{isotopic mass x relative abundance})}{\text{total relative abundance}}$$

If relative abundance is used instead of percentage abundance use this equation

Example 5: Calculate the relative atomic mass of Tellurium from the following abundance data: 124-Te relative abundance 2; 126-Te relative abundance 4; 128-Te relative abundance 7; 130-Te relative abundance 6

$$\text{R.A.M} = \frac{[(124\text{x}2) + (126\text{x}4) + (128\text{x}7) + (130\text{x}6)]}{19}$$
$$= 127.8$$

Example 6: Copper has two isotopes 63-Cu and 65-Cu. The relative atomic mass of copper is 63.5. Calculate the percentage abundances of these two isotopes.

63.55 = y*x*63 + (1-y)*x*65
63.55 = 63y +65 -65y
63.55 = 65 -2y
2y = 1.45
y = 0.725

%abundance 63-Cu =72.5% %abundance 65-Cu = 27.5%

Empirical formulae

Definition: An empirical formula is the **simplest** ratio of atoms of each **element** in the compound.

General method

Step 1 : Divide each mass (or % mass) by the atomic mass of the element

Step 2 : For each of the answers from step 1 divide by the smallest one of those numbers.

Step 3: sometimes the numbers calculated in step 2 will need to be multiplied up to give whole numbers.

These whole numbers will be the empirical formula.

The same method can be used for the following types of data:

1. masses of each element in the compound
2. percentage mass of each element in the compound

Example 7 : Calculate the empirical formula for a compound that contains 1.82g of K, 5.93g of I and 2.24g of O

Step1: Divide each mass by the atomic mass of the element to give moles

K = 1.82 / 39.1	I = 5.93/126.9	O = 2.24/16
= 0.0465 mol	= 0.0467mol	= 0.14mol

Step 2 For each of the answers from step 1 divide by the smallest one of those numbers.

K = 0.0465/0.0465	I = 0.0467/0.0465	O = 0.14 / 0.0465
=1	= 1	= 3

Empirical formula =KIO_3

Molecular formula from empirical formula

Definition: A molecular formula is the **actual** number of atoms of each element in the compound.

From the relative molecular mass (*M*r) work out how many times the mass of the empirical formula fits into the *M*r.

Example 8 : work out the molecular formula for the compound with an empirical formula of C_3H_6O and a M_r of 116

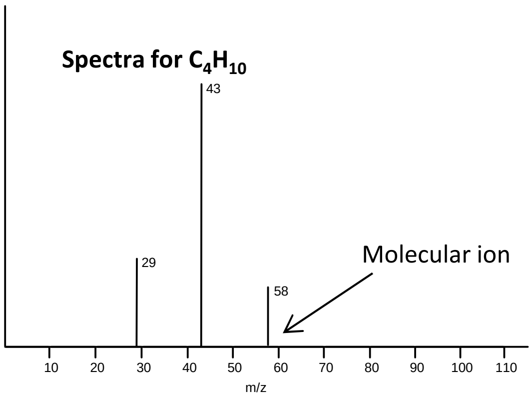
C_3H_6O has a mass of 58

The empirical formula fits twice into M_r of 116

So molecular formula is $C_6H_{12}O_2$

The Mr does not need to be exact to turn an empirical formula into the molecular formula because the molecular formula will be a whole number multiple of the empirical formula

Remember the *M*r of a substance can be found out from using a mass spectrometer. The molecular ion (the peak with highest m/z) will be equal to the *M*r.



Combustion Analysis for Calculating Empirical Formula

Example 9
0.328 g of a compound containing C,H and O was burnt completely in excess oxygen, producing 0.880 g of carbon dioxide and 0.216 g of water. Use these data to calculate the empirical formula of the compound.

Work out moles of CO_2 = Mass of CO_2/*M*r of CO_2
= 0.88/44
=0.02mol

Moles of C in compound = moles of CO_2
= 0.02 mol → Mass of C in compound = mol of C x 12
=0.02 x12
=0.24g

Work out moles of H_2O = Mass of H_2O /*M*r of H_2O
= 0.216/18
=0.012mol

Moles of H in compound = 2 x moles of H_2O
= 0.024 mol → Mass of H in compound = mol of H x 1
=0.024 x1
=0.024g

Work out mass of O in compound = mass of compound – mass of C – mass of H
= 0.328 – 0.24 -0.024
=0.064

Work out moles of O in compound = Mass of O /*A*r of O
= 0.064/16
= mol 0.004

Work out molar ratio of 3 elements (divide by smallest moles)

C = 0.02/0.004
=5

H = 0.024/0.004
=6

O = 0.004/0.004
= 1

empirical formula = C_5H_6O

Molar Gas Volume

1 mole of any gas at room pressure (1atm) and room temperature 25°C will have the volume of 24dm^3

Example 10 : Calculate the volume in dm^3 at room temperature and pressure of 50.0g of Carbon dioxide gas ?

amount = mass/*M*r
= 50/ (12 + 16 x2)
= 1.136 mol

Gas Volume (dm^3)= amount x 24
= 1.136 x 24
= or 27.3 dm^3 to 3 sig fig

For most calculations at A-level use the following 3 equations to calculate amount in moles

Learn these equations carefully and what units to use in them.

1. For pure solids, liquids and gases

moles = $\frac{\text{mass}}{Mr}$

Unit of Mass: grams
Unit of moles : mol

Remember the *Mr* must be calculated and quoted to 1dp

2. For gases

Gas Volume (dm^3)= amount x 24

This equation gives the volume of a gas at room pressure (1atm) and room temperature 25°C.

PV = nRT

Unit of Pressure (P):Pa
Unit of Volume (V): **m^3**
Unit of Temp (T): K
n= moles
R = 8.31

Converting temperature

°C → K add 273

Note the different units for volume

3. For solutions

Concentration = $\frac{\text{moles}}{\text{volume}}$

Unit of concentration: mol dm^{-3} or M
Unit of Volume: **dm^3**

Converting volumes

cm^3 → dm^3 ÷ 1000
cm^3 → m^3 ÷ 1000 000
dm^3 → m^3 ÷ 1000

Significant Figures

Give your answers to the same number of significant figures as the number of significant figures for the data you given in a question. If you are given a mixture of different significant figures, use the smallest

Density, ρ

Density calculations are usually used with pure liquids but to work out the mass from a measured volume. It can also be used with solids and gases.

density = $\frac{\text{mass}}{\text{Volume}}$

Density is usually given in g cm^{-3} but can be kg m^{-3}, g dm^{-3}
Care needs to be taken if different units are used.

Example 11 : How many molecules of ethanol are there in a 0.500 dm^3 of ethanol (CH_3CH_2OH) liquid ? The density of ethanol is 0.789 g cm^{-3}

Mass = density x Volume
ethanol
= 0.789 x 500
= 394.5g

moles = mass/*Mr*
= 394.5/ 46.0
= 8.576 mol

Number of molecules= moles x 6.022 x 10^{23}
= 8.576 x 6.022 x 10^{23}
= 5.16 x10^{24}(to 3 sig fig)

Example 12 : There are 980mol of pure gold in a bar measuring 10 cm by 20 cm by 50 cm. What is the density of gold in kg dm^{-3}

Mass = moles x *Mr*
= 980 x 197
= 193060 g
= 193.06kg

Volume = 10x20x50
= 10 000cm^3
= 10dm^3

density = mass/volume
= 193/10
= 19.3 kg dm^{-3}

Hydrated salt

A Hydrated salt contains water of crystallisation

$Cu(NO_3)_2 \cdot 6H_2O$

hydrated copper (II) nitrate(V).

$Cu(NO_3)_2$

Anhydrous copper (II) nitrate(V).

Example 13
$Na_2SO_4 \cdot xH_2O$ has a molar mass of 322.1, Calculate the value of x
Molar mass xH_2O = 322.1 – (23x2 + 32.1 + 16x4)
= 180
X = 180/18
=10

Heating in a crucible

This method could be used for measuring mass loss in various thermal decomposition reactions and also for mass gain when reacting magnesium in oxygen.

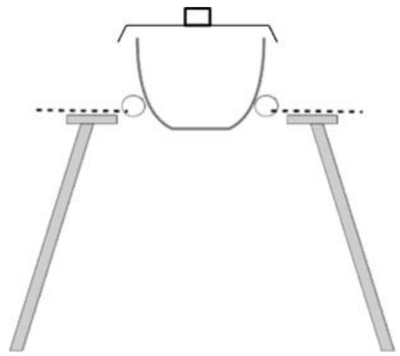
The water of crystallisation in calcium sulphate crystals can be removed as water vapour by heating as shown in the following equation.

$CaSO_4.xH_2O(s) \rightarrow CaSO_4(s) + xH_2O(g)$

Method.

- Weigh an empty clean dry crucible and lid .
- Add 2g of hydrated calcium sulphate to the crucible and weigh again
- Heat strongly with a Bunsen for a couple of minutes
- Allow to cool
- Weigh the crucible and contents again
- Heat crucible again and reweigh until you reach a constant mass (do this to ensure reaction is complete).

The lid improves the accuracy of the experiment as it prevents loss of solid from the crucible but should be loose fitting to allow gas to escape.



Large amounts of hydrated calcium sulphate, such as 50g, should not be used in this experiment as the decomposition is likely to be incomplete.

The crucible needs to be dry otherwise a wet crucible would give an inaccurate result. It would cause mass loss to be too large as the water would be lost when heating.

Small amounts of the solid , such as 0.100 g, should **not** be used in this experiment as the percentage uncertainties in weighing will be too high.

Example 14. 3.51 g of hydrated zinc sulphate were heated and 1.97 g of anhydrous zinc sulphate were obtained.
Use these data to calculate the value of the integer *x* in $ZnSO_4.xH_2O$

Calculate the mass of H_2O = 3.51 – 1.97 = 1.54g

Calculate moles of $ZnSO_4$ $= \frac{1.97}{161.5}$

= 0.0122

Calculate moles of H_2O $= \frac{1.54}{18}$

= 0.085

Calculate ratio of mole of $ZnSO_4$ to H_2O $= \frac{0.0122}{0.0122}$ $= \frac{0.085}{0.0122}$

= 1 = 7

X = 7

Concentration of Solutions

A solution is a mixture formed when a solute dissolves in a solvent. In chemistry we most commonly use water as the solvent to form aqueous solutions. The solute can be a solid, liquid or a gas.

Molar concentration can be measured for solutions. This is calculated by dividing the amount in moles of the solute by the volume of the solution. The volume is measure is dm^3. The unit of molar concentration is mol dm^{-3} ; it can also be called molar using symbol M

Concentration = $\frac{\text{moles}}{\text{volume}}$

Unit of concentration: mol dm^{-3} or M
Unit of Volume: **dm^3**

Converting volumes

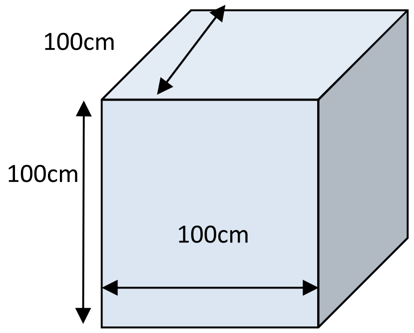
A m^3 is equivalent to a cube 100cmx100cmx100cm= 1000000cm^3

A dm^3 is equivalent to a cube 10cmx10cmx10cm= 1000cm^3

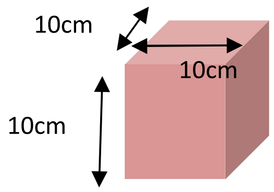
1dm^3 = 1litre

A cm^3 is equivalent to a cube 1cmx1cmx1cm

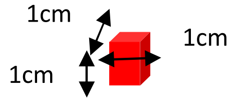
1cm^3 = 1 ml



1m^3



1dm^3 or 1 litre



1cm^3

1 m^3 = 1000 dm^3 or 1000L
To convert m^3 into dm^3 multiply by 1000

1 dm^3 = 1000 cm^3 or 1000mL
To convert cm^3 into dm^3 divide by 1000

$cm^3 \rightarrow dm^3 \div 1000$
$cm^3 \rightarrow m^3 \div 1000\ 000$
$dm^3 \rightarrow m^3 \div 1000$

Example 15 What is the concentration of solution made by dissolving 5.00g of Na_2CO_3 in 250 cm^3 water?

moles = mass/*Mr*

= 5 / (23.0 x2 + 12 +16 x3)

= 0.0472 mol

conc= moles/Volume

= 0.0472 / **0.25**

= 0.189 mol dm^{-3}

Example 16 What is the concentration of solution made by dissolving 10kg of Na_2CO_3 in 0.50 m^3 water?

moles = mass/*Mr*

= 10 000 / (23.0 x2 + 12 +16 x3)

= 94.2 mol

conc= moles/Volume

= 94.2 / **500**

= 0.19 mol dm^{-3}

Mass Concentration

The concentration of a solution can also be measured in terms of mass of solute per volume of solution

Mass Concentration = $\frac{\text{mass}}{\text{volume}}$

Unit of mass concentration: g dm^{-3}
Unit of Mass **g**
Unit of Volume: **dm^3**

To turn concentration measured in mol dm^{-3} into concentration measured in g dm^{-3} multiply by *M*r of the substance
conc in g dm^{-3} = conc in mol dm^{-3} x *M*r
The concentration in g dm^{-3} is the same as the mass of solute dissolved in 1dm^3

Ions dissociating

When soluble ionic solids dissolve in water they will dissociate into separate ions. This can lead to the concentration of ions differing from the concentration of the solute.

Example 17

If 5.86g (0.1 mol) of sodium chloride (NaCl) is dissolved in 1 dm^3 of water then the concentration of sodium chloride solution would be 0.1moldm^{-3} .
However the 0.1mol sodium chloride would split up to form 0.1 mol of sodium ions and 0.1 mol of chloride ions. The concentration of sodium ions is therefore 0.1 mol dm^{-3} and the concentration of chloride ions is also 0.1 mol dm^{-3}

$NaCl(s) + aq \rightarrow Na^+(aq) + Cl^-(aq)$

0.1mol 0.1mol 0.1mol

Example 18

If 9.53g (0.1 mol) of magnesium chloride ($MgCl_2$) is dissolved in 1 dm^3 of water then the concentration of magnesium chloride solution ($MgCl_2$ aq) would be 0.1moldm^{-3} .
However the 0.1mol magnesium chloride would split up to form 0.1 mol of magnesium ions and 0.2 mol of chloride ions. The concentration of magnesium ions is therefore 0.1 mol dm^{-3} and the concentration of chloride ions is now 0.2 mol dm^{-3}

$MgCl_2(s) + aq \rightarrow Mg^{2+}(aq) + 2Cl^-(aq)$

0.1mol 0.1mol 0.2mol

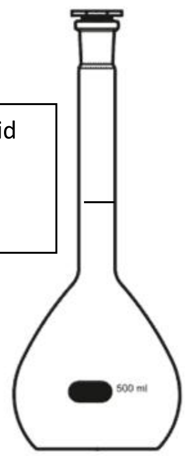
Making a solution

- Weigh the sample bottle containing the required mass of solid on a 2 dp balance
- Transfer to beaker and reweigh sample bottle
- Record the difference in mass

Alternatively the known mass of solid in the weighing bottle could be transferred to beaker, washed and washings added to the beaker.

• Add 100cm^3 of distilled water to the beaker. Use a glass rod to stir to help dissolve the solid.

•Sometimes the substance may not dissolve well in cold water so the beaker and its contents could be heated gently until all the solid had dissolved.



- Pour solution into a 250cm^3 graduated flask via a funnel.
- Rinse beaker and funnel and add washings from the beaker and glass rod to the volumetric flask.
- make up to the mark with distilled water using a dropping pipette for last few drops.
- Invert flask several times to ensure uniform solution.

Remember to fill so the bottom of the meniscus sits on the line on the neck of the flask. With dark liquids like potassium manganate it can be difficult to see the meniscus.

Dilutions

Diluting a solution

- Pipette 25cm^3 of original solution into a 250cm^3 volumetric flask
- make up to the mark with distilled water using a dropping pipette for last few drops.
- Invert flask several times to ensure uniform solution.

Using a volumetric pipette is more accurate than a measuring cylinder because it has a smaller uncertainty

Use a teat pipette to make up to the mark in volumetric flask to ensure volume of solution accurately measured and one doesn't go over the line

Calculating Dilutions

Diluting a solution will not change the amount of moles of solute present but increase the volume of solution and hence the concentration will lower

moles= volume x concentration

If amount of moles does not change then
Original volume x original concentration = new diluted volume x new diluted concentration

so

$$\text{new diluted concentration} = \text{original concentration} \times \frac{\text{Original volume}}{\text{new diluted volume}}$$

The new diluted volume will be equal to the original volume of solution added + the volume of water added.

Example 19

If 50 cm^3 of water are added to 150 cm^3 of a 0.20 mol dm^{-3} NaOH solution, what will the concentration of the diluted solution be?

$$\text{new diluted concentration} = \text{original concentration} \times \frac{\text{Original volume}}{\text{new diluted volume}}$$

$$\text{new diluted concentration} = 0.20 \times \frac{0.150}{0.200}$$

$$= 0.15 \text{ mol dm}^{-3}$$

Example 20

Calculate the volume of water in cm^3 must be added to dilute 5.00 cm^3 of 1.00 mol dm^{-3} hydrochloric acid so that it has a concentration of 0.050 mol dm^{-3} ?

Moles original solution = conc x vol
= 1.00 x 0.005
= 0.005

New volume = moles /conc
= 0.005/0.05
= 0.1dm^3 = 100cm^3

Volume of water added = 100 - 5 = 95cm^3

Safety and hazards

Irritant - dilute acid and alkalis- wear googles
Corrosive- stronger acids and alkalis wear goggles
Flammable – keep away from naked flames
Toxic – wear gloves- avoid skin contact- wash hands after use
Oxidising- Keep away from flammable / easily oxidised materials

Hazardous substances in low concentrations or amounts will not pose the same risks as the pure substance.

Converting quantities between different substances using a balanced equation

$N_2 + 3H_2 \rightarrow 2NH_3$

The balancing (stoichiometric) numbers are mole ratios
e.g. 1 mole of N_2 reacts with 3 moles of H_2 to produce 2moles of NH_3

Typically the quantity of one substance is given and you are asked to calculate a quantity for another substance in the reaction. Any of the above three equations can be used.

1. For pure solids, liquids and gases

moles = $\frac{\text{mass}}{Mr}$

2. For gases

PV = nRT

Or use the molar gas volume
1 mol gas =24dm^3 at RTP

3. For solutions

Concentration = $\frac{\text{moles}}{\text{volume}}$

Step 1:
Use one of the above 3 equations to convert any given quantity into moles
Mass→ moles
PVT of gas → moles
Conc and vol of solution → moles

→

Step 2:
Use balanced equation to convert moles of initial substance into moles of second substance

→

Step 3
Convert moles of second substance into quantity question asked for using relevant equation
e.g. Moles ,*Mr* → mass
Mole, P, T gas → vol gas
Moles, vol solution → conc

Example 21: What mass of Carbon dioxide would be produced from heating 5.50 g of sodium hydrogencarbonate?
$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$

Step 1: work out moles of sodium hydrogencarbonate
Moles = mass / Mr
= 5.50 /84
= 0.0655 mol

Step 2: use balanced equation to give moles of CO_2
2 moles $NaHCO_3$: 1 moles CO_2
So 0.0655 HNO_3 : 0.0328mol CO_2

Step 3: work out mass of CO_2
Mass = moles x *Mr*
= 0.0328 x 44.0
=1.44g

Example 22: 23.6cm^3 of H_2SO_4 neutralised 25.0cm^3 of 0.150M NaOH. What is the concentration of the H_2SO_4?
$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$

Step 1: work out moles of sodium hydroxide
Moles = conc x vol
= 0.150 x 0.025
= 0. 00375 mol

Step 2: use balanced equation to give moles of H_2SO_4
2 moles NaOH : 1 moles H_2SO_4
So 0.00375 NaOH : 0.001875 mol H_2SO_4

Step 3 work out concentration of H_2SO_4

conc= moles/Volume

= 0.001875 / 0.0236

= 0.0794 mol dm^{-3}

Example 23: What is the total volume of gas produced in dm^3 at 333K and 100kPa when 0.651 g of magnesium nitrate decomposes when heated?
$2Mg(NO_3)_{2\,(s)} \rightarrow 2MgO_{(s)} + 4NO_{2\,(g)} + O_{2\,(g)}$

Step 1: work out moles of magnesium nitrate
Moles = mass / *Mr*
= 0.651 / 148.3
= 0.00439 mol

Step 2: use balanced equation to give moles of gas produced
2 moles $Mg(NO_3)_2$: $4NO_{2\,(g)} + O_{2\,(g)}$ ie 5moles of gas
So 0.00439 $Mg(NO_3)_2$: 0.01098(0.00439 x $^5/_2$) moles gas

Step 3: work out volume of gas
Volume = nRT/P
= (0.01098 x 8.31 x 333)/ 100000
= 0.000304m^3
= 0.303dm^3

Example 24: What mass of Copper would react completely with 150 cm^3 of 1.60M nitric acid?
$3Cu + 8HNO_3 \rightarrow 3Cu(NO_3)_2 + 2NO + 4H_2O$

Step 1: work out moles of nitric acid
Moles = conc x vol
= 1.6 x 0.15
= 0.24 mol

Step 2: use balanced equation to give moles of Cu
8 moles HNO_3 : 3 moles Cu
So 0.24 HNO_3 : 0.09 (0.24 x $^3/_8$) mol Cu

Step 3: work out mass of Cu
Mass = moles x *Mr*
= 0.09 x 63.5
=5.71g

Limiting and excess reactants

Example 25 Calculate the maximum mass of titanium that could be produced from reacting 100 g of $TiCl_4$ with 80 g of sodium

$TiCl_4 + 4\ Na \rightarrow 4\ NaCl + Ti$

Step 1: work out amount, in mol, $TiCl_4$
amount = mass / *M*r
= 100 /189.9
= 0.527 mol

Step 1: work out amount, in mol, Na
amount = mass / *M*r
= 80/23.0
= 3.48 mol

Step 2 use balanced equation to work out which reactant is in excess
Using $1TiCl_4$:4 Na ratio we can see that 0.527mol of $TiCl_4$ should react with 2.108 mol of Na. We actually have 3.48 mole of Na which is an excess of 1.372 moles. We can complete calculation using the limiting reactant of $TiCl_4$

Step 3: use balanced equation to work out amount in mol of Ti formed
1 mol $TiCl_4$: 1 mole Ti
So 0.527mol $TiCl_4$ produces 0.527 mole Ti

Step 4: work out mass of Ti formed
Mass = amount x Mr
= 0.527 x 47.9
=25.24g

% Yield

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

Example 26: 25.0g of Fe_2O_3 was reacted and it produced 10.0g of Fe. Calculate the percentage yield?

$Fe_2O_3 + 3CO \rightarrow 2Fe + 3\ CO_2$

First calculate maximum mass of Fe that could be produced

Step 1: work out moles of Iron oxide
Moles = mass / *M*r
=25.0 / 159.6
= 0.1566 mol

Step 2: use balanced equation to give moles of Fe
1 moles Fe_2O_3 : 2 moles Fe
So 0.1566 Fe_2O_3 : 0.313moles Fe

Step 3: work out mass of Fe
Mass = moles x *A*r
= 0.313 x 55.8
=17.5g

Step 4 : calculate %yield

% yield = (actual yield/theoretical yield) x 100

= (10/ 17.5) x 100
= 57.1%

Titrations

The method for carrying out the titration

•**rinse equipment** (burette with acid, pipette with alkali, conical flask with distilled water)
•**pipette 25 cm^3 of alkali into conical flask**
•**touch surface of alkali with pipette** (to ensure correct amount is added)
•**adds acid solution from burette**
•**make sure the jet space** in the burette **is filled** with acid
•add **a few drops of indicator** and refer to colour change at end point
•phenolphthalein [pink (alkali) to colourless (acid): end point pink colour just disappears] [use if NaOH is used]
•methyl orange [yellow (alkali) to red (acid): end point orange] [use if HCl is used]
•use a white tile underneath the flask to help observe the colour change
•add acid to alkali whilst **swirling the mixture** and **add acid dropwise at end point**
•**note burette reading** before and after addition of acid
•**repeats titration** until **at least 2 concordant results** are obtained- two readings within 0.1 of each other

Safety precautions

Acids and alkalis are corrosive
(at low concentrations acids are irritants)
Wear eye protection and gloves
If spilled immediately wash affected parts after spillage

If substance is unknown treat it as potentially toxic and wear gloves.

If the jet space is not filled properly prior to commencing the titration it will lead to errors if it then fills during the titration, leading to a larger than expected titre reading.

A conical flask is used in preference to a beaker because it is easier to swirl the mixture in a conical flask without spilling the contents.

Indicators are generally weak acids so we only add a few drops of them. If too much is added it will affect the titration result

Working out average titre results
Only make an average of the concordant titre results

If **2 or 3 values are within 0.10cm^3** and therefore **concordant** or close then we can say results are accurate and **repeatable** and **the titration technique is good/ consistent**

Distilled water can be added to the conical flask during a titration to wash the sides of the flask so that all the acid on the side is washed into the reaction mixture to react with the alkali.
It does not affect the titration reading as water does not react with the reagents or change the number of moles of acid added.

Recording results
•Results should be clearly recorded in a table
•Result should be recorded in full (i.e. both initial and final readings)
•**Record titre volumes to 2dp (0.05 cm^3)**

Common Titration Equations

$CH_3CO_2H + NaOH \rightarrow CH_3CO_2^-Na^+ + H_2O$

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

$HCl + NaOH \rightarrow NaCl + H_2O$

$NaHCO_3 + HCl \rightarrow NaCl + CO_2 + H_2O$

$Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$

Titrating mixtures
If titrating a mixture to work out the concentration of an active ingredient it is necessary to consider if the mixture contains other substances that have acid base properties.
If they don't have acid base properties we can titrate with confidence.

Testing batches
In quality control it will be necessary to do titrations/testing on several samples as the amount/concentration of the chemical being tested may vary between samples.

Safely dealing with excess acid
Sodium hydrogen carbonate ($NaHCO_3$) and calcium carbonate ($CaCO_3$) are good for neutralising excess acid in the stomach or acid spills because they are not corrosive and will not cause a hazard if used in excess. They also have no toxicity if used for indigestion remedies but the CO_2 produced can cause wind.
Magnesium hydroxide is also suitable for dealing with excess stomach acid as it has low solubility in water and is only weakly alkaline so not corrosive or dangerous to drink (unlike the strong alkali sodium hydroxide). It will also not produce any carbon dioxide gas.

More complicated titration calculations- taking samples

Example 27: A 25.0cm^3 sample of vinegar was diluted in a 250cm^3 volumetric flask. This was then put in a burette and 23.10cm^3 of the diluted vinegar neutralised 25.0 cm^3 of 0.100M NaOH. What is the concentration of the vinegar in gdm^{-3} ?

$CH_3CO_2H + NaOH \rightarrow CH_3CO_2^-Na^+ + H_2O$

Step 1: work out moles of sodium hydroxide
moles = conc x vol
= 0.10 x 0.025
= 0. 00250 mol

Step 2: use balanced equation to give moles of CH_3CO_2H
1 moles NaOH : 1 moles CH_3CO_2H
So 0.00250 NaOH : 0.00250 mol CH_3CO_2H

Step 3 work out concentration of diluted CH_3CO_2H in 23.1 (and 250 cm^3) in moldm^{-3}

conc= moles/Volume

= 0.00250 / 0.0231

= 0.108 mol dm^{-3}

Step 4 work out concentration of original concentrated CH_3CO_2H in 25cm^3 in moldm^{-3}

conc = 0.108 x 10 = 1.08 mol dm^{-3}

Step 5 work out concentration of CH_3CO_2H in original concentrated 25 cm^3 in gdm^{-3}

conc in gdm^{-3} = conc in mol dm^{-3} x *Mr*

= 1.08 x 60 = 64.8 g dm^{-3}

Example 28. An unknown metal carbonate reacts with hydrochloric acid according to the following equation.
$M_2CO_3(aq) + 2HCl(aq) \rightarrow 2MCl(aq) + CO_2(g) + H_2O(l)$
A 3.96 g sample of M_2CO_3 was dissolved in distilled water to make 250 cm^3 of solution. A 25.0 cm^3 portion of this solution required 32.8 cm^3 of 0.175 mol dm^{-3} hydrochloric acid for complete reaction. Calculate the *Mr* of M_2CO_3 and identify the metal M

1. Calculate the number of moles of HCl used
moles = conc x vol
= 0.175 x 0.0328
= 0. 00574 mol

2. Work out number of moles of M_2CO_3 in 25.0 cm^3 put in conical flask
use balanced equation to give moles of M_2CO_3
2 mol HCl : 1 mol M_2CO_3
So 0. 00574 NaOH : 0.00287 moles M_2CO_3

3. Calculate the number of moles M_2CO_3 acid in original 250 cm^3 of solution

Moles in 250cm^3 = 0.00287 x10
=0.0287

4. work out the *Mr* of M_2CO_3

Mr = mass / moles

= 3.96/ 0.0287= 138.0

5. Work out *Ar* of M = $\frac{(138-12- 16x3)}{2}$

Ar of M = 39   M= potassium

Common Titration Equations

$CH_3CO_2H + NaOH \rightarrow CH_3CO_2^-Na^+ + H_2O$

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

$HCl + NaOH \rightarrow NaCl + H_2O$

$NaHCO_3 + HCl \rightarrow NaCl + CO_2 + H_2O$

$Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$

Example 29

950 mg of impure calcium carbonate tablet was crushed. 50.0 cm^3 of 1.00 mol dm^{-3} hydrochloric acid, an excess, was then added. After the tablet had reacted, the mixture was transferred to a volumetric flask. The volume was made up to exactly 100 cm^3 with distilled water. 10.0 cm^3 of this solution was titrated with 11.1cm^3 of 0.300 mol dm^{-3} sodium hydroxide solution.
What is the percentage of $CaCO_3$ by mass in the tablet?

1. Calculate the number of moles of sodium hydroxide used

moles= conc x vol
= 0.30 x 0.0111
= 0. 00333 mol

2. Work out number of moles of hydrochloric acid left in 10.0 cm^3
use balanced equation to give moles of HCl
1 mol NaOH : 1 mol HCl
So 0.00333 NaOH : 0.00333 moles HCl

3. Calculate the number of moles of hydrochloric acid left in 100 cm^3 of solution

Moles in 100cm^3 = 0.00333 x10
=0.0333

4. Calculate the number of moles of HCl that reacted with the indigestion tablet.

In original HCl 50.0 cm^3 of 1.00 mol dm^{-3} there is 0.05moles

moles of HCl that reacted with the indigestion tablet. =0.05 -0.0333
=0.0167

5 Use balanced equation to give moles of $CaCO_3$
$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$
2 mol HCl : 1 mol $CaCO_3$
So 0.0167 HCl : 0.00835 moles $CaCO_3$

6. work out the mass of $CaCO_3$ in original tablet

mass= moles x *Mr*

= 0.00835 x 100 = 0.835 g

percentage of $CaCO_3$ by mass in the tablet = 0.835/0.950 x100

= 87.9 %

Uncertainty

Readings and Measurements

Readings
the values found from a single judgement when using a piece of equipment

Measurements
the values taken as the difference between the judgements of two values (e.g. using a burette in a titration)

The uncertainty of a reading (one judgement) is at least ± 0.5 of the smallest scale reading.
The uncertainty of a measurement (two judgements) is at least ± 1 of the smallest scale reading.

Calculating Apparatus Uncertainties
Each type of apparatus has a sensitivity uncertainty

•balance $\pm$ 0.001 g
•volumetric flask $\pm$ 0.1 cm^3
•25 cm^3 pipette $\pm$ 0.1 cm^3
•burette (start & end readings and end point) $\pm$ 0.15 cm^3

Calculate the percentage error for each piece of equipment used by

$$\% \text{ uncertainty} = \pm \frac{\text{uncertainty}}{\text{Measurement made on apparatus}} \times 100$$

e.g. for burette
% uncertainty = 0.15/average titre result x100

To calculate the maximum total percentage apparatus uncertainty in the final result add all the individual equipment uncertainties together.

To decrease the apparatus uncertainties you can either decrease the sensitivity uncertainty by using apparatus with a greater resolution (finer scale divisions) or you can increase the size of the measurement made.

Uncertainty of a measurement using a burette. If the burette used in the titration had an uncertainty for each reading of +/– 0.05 cm^3 then during a titration two readings would be taken so the uncertainty on the titre volume would be +/– 0.10 cm^3 . Then often another 0.05 is added on because of uncertainty identifying the end point colour change

Reducing uncertainties in a titration

Replacing measuring cylinders with pipettes or burettes which have lower apparatus uncertainty will lower the error

To reduce the uncertainty in a burette reading it is necessary to make the titre a larger volume. This could be done by: increasing the volume and concentration of the substance in the conical flask or by decreasing the concentration of the substance in the burette.

If looking at a series of measurements in an investigation the experiments with the smallest readings will have the highest experimental uncertainties.

Reducing uncertainties in measuring mass
Using a more accurate balance or a larger mass will reduce the uncertainty in weighing a solid
Weighing sample before and after addition and then calculating difference will ensure a more accurate measurement of the mass added.

Calculating the percentage difference between the actual value and the calculated value

If we calculated an *M*r of 203 and the real value is 214, then the calculation is as follows:
Calculate difference 214-203 = 11
% = 11/214 x100
=5.41%

If the %**uncertainty** due to the apparatus **<** percentage difference between the actual value and the calculated value then there is a discrepancy in the result due to other errors.

If the %**uncertainty** due to the apparatus **>** percentage difference between the actual value and the calculated value then there is no discrepancy and all errors in the results can be explained by the sensitivity of the equipment.