2.1.3 Amount of substance

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.

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

DEFINITION: **Molar mass** is the mass in grams of 1 mole of a substance and is given the unit of g mol^{-1}

Molar Mass for a compound can be calculated by adding up the mass numbers(from the periodic table) of each element in the compound
eg $CaCO_3$ = 40.1 + 12.0 +16.0 x3 = 100.1

Molar gas volume (gas volume per mole, units dm^3 mol^{-1}) . This is the volume of 1 mole of a gas at a given temperature and pressure. All gases have this same volume. At room pressure (1atm) and room temperature 25°C the molar gas volume is 24 dm^3 mol^{-1}

Avogadro's constant
There are 6.02×10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.02×10^{23} of that entity':

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

1 mole of copper atoms will contain 6.02×10^{23} atoms
1 mole of carbon dioxide molecules will contain 6.02×10^{23} molecules
1 mole of sodium ions will contain 6.02×10^{23} ions

For pure solids, liquids and gases

$$\text{Amount in mol} = \frac{\text{mass}}{Mr}$$

Unit of mass: grams
Unit of amount : mol

Example 1: Calculate the amount, in mol, in 35.0g of $CuSO_4$

amount = mass/*Mr*
= 35/ (63.5 + 32 +16 x4)
= 0.219 mol

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

Example 2: Calculate the amount, in mol, in 75.0mg of $CaSO_4.2H_2O$

amount = mass/*Mr*
= 0.075/ (40 + 32.0 +16.0 x4 + 18.0x2)
= 4.36×10^{-4} mol

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

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

Step1: Calculate amount, in mol, by dividing each mass by the atomic mass of the element

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

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 4. Deduce 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 the molecular formula is $C_6H_{12}O_2$

The *M*r 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

Hydrated salt

A Hydrated salt contains water of crystallisation

$Cu(NO_3)_2 . 6H_2O$

hydrated copper (II) nitrate(V).

$Cu(NO_3)_2$

Anhydrous copper (II) nitrate(V).

Example 5

$Na_2SO_4 . xH_2O$ 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 sulfate 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 sulfate to the crucible and weigh again

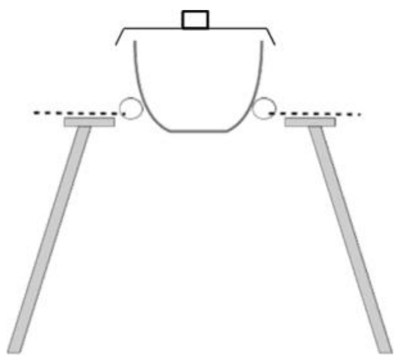
•Heat strongly with a Bunsen for a couple of minutes

•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 like to be incomplete.

Small amounts the solid , such as 0.100 g, should **not** be used in this experiment as errors in weighing are too high.

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 water would be lost when heating.

Example 6. . 3.51 g of hydrated zinc sulfate were heated and 1.97 g of anhydrous zinc sulfate were obtained.

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 $ZnSO_4$ $= \frac{1.97}{161.5}$ $= 0.0122$ mol

Calculate moles of H_2O $= \frac{1.54}{18}$ $=0.085$ mol

Calculate ratio of mole of $ZnSO_4$ to H_2O $= \frac{0.0122}{0.0122}$ $=1$

$= \frac{0.085}{0.0122}$ $=7$

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.

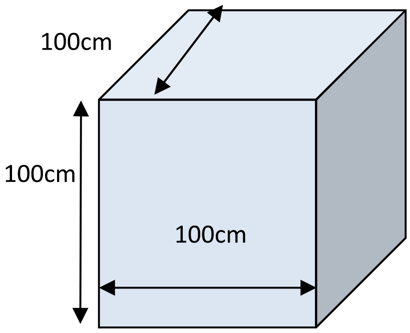
Molar concentration can be measured for solutions. This is calculated by dividing the amount in moles of the solute by the volume of the solution. The volume is measure is dm^3. The unit of molar concentration is mol dm^{-3} ; it can also be called molar using symbol M

$$\boxed{\textbf{Concentration} = \frac{\textbf{amount}}{\textbf{volume}}}$$

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

Converting volumes

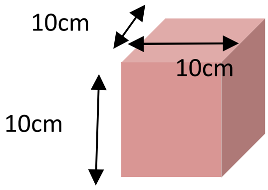
A m^3 is equivalent to a cube 100cmx100cmx100cm= 1000000 cm^3



$1m^3$

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

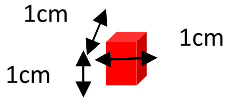
$1dm^3$ = 1litre



$1dm^3$ or 1 litre

A cm^3 is equivalent to a cube 1cmx1cmx1cm

$1cm^3$ = 1 mL



$1cm^3$

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 7 Calculate the concentration of solution made by dissolving 5.00 g of Na_2CO_3 in 250 cm^3 water

amount = mass/*Mr*

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

= 0.0472 mol

conc= amount/volume

= 0.0472 / **0.25**

= 0.189 mol dm^{-3}

Example 8 Calculate the concentration of solution made by dissolving 10 kg of Na_2CO_3 in 0.50 m^3 water

amount = mass/*Mr*

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

= 94.2 mol

conc= amount/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

$$\text{mass concentration} = \frac{\text{mass}}{\text{volume}}$$

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 9

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 0.1 mol dm^{-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 10

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 0.1 mol dm^{-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

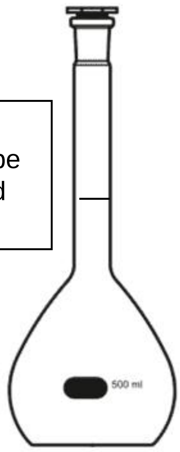
- Weigh the sample bottle containing the required mass of solid on a 2 dp balance
- Transfer to beaker and reweigh sample bottle
- Record the difference in mass

• 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.

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



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 $25 cm^3$ of original solution into a $250 cm^3$ 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

amount= 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 11
$50 cm^3$ of water are added to $150 cm^3$ of a $0.20 mol dm^{-3}$ NaOH solution. Calculate the concentration of the diluted solution.

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

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

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

Example 12
Calculate the volume of water in cm^3 that must be added to dilute $5.00 cm^3$ of $1.00 mol dm^{-3}$ hydrochloric acid so that it has a concentration of $0.050 mol dm^{-3}$

Amount in mol original solution = conc x vol
= 1.00 x 0.005
= 0.005

New volume = amount /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.

Ideal Gas Equation

The ideal gas equation applies to all gases and mixtures of gases. If a mixture of gases is used the value n will be the total moles of all gases in the mixture.

PV = nRT

Unit of Pressure (P):Pa
Unit of Volume (V): $\mathbf{m^3}$
Unit of Temp (T): K
n= moles
R = 8.31 $JK^{-1}mol^{-1}$

The biggest problems students have with this equation is choosing and converting to the correct units, so pay close attention to the units.

Example 13: Calculate the mass of Cl_2 gas that has a pressure of 100 kPa, temperature 20 °C , volume 500 cm^3. (R = 8.31)

moles = PV/RT

= 100 000 x 0.0005 / (8.31 x 293)

= 0.0205 mol

100 kPa = 100 000 Pa
20°C = 20+273= 293K
500 cm^3 = 0.0005 m^3

Mass = amount x *M*r
= 0.0205 x (35.5 x2)
= 1.46 g

Converting temperature

°C → K add 273

Example 14: 0.150g of a volatile liquid was injected into a sealed gas syringe. The gas syringe was placed in an oven at 70°C at a pressure of 100kPa and a volume of 80cm^3 was measured. Calculate the *M*r of the volatile liquid (R =8.31)

moles = PV/RT

= 100 000 x 0.00008 / (8.31 x 343)

= 0.00281 mol

100 kPa = 100 000 Pa
80 cm^3 = 0.00008 m^3

*M*r = mass/amount
= 0.15 / 0.00281
= 53.4 g mol^{-1}

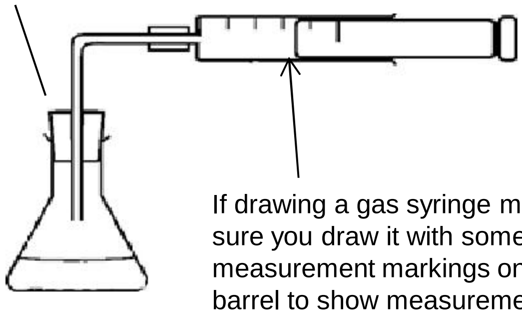
Using a gas syringe

Gas syringes can be used for a variety of experiments where the volume of a gas is measured, possibly to work out moles of gas or to follow reaction rates.

The volume of a gas depends on pressure and temperature so when recording volume it is important to note down the temperature and pressure of the room.

Moles of gas can be calculated from gas volume (and temperature and pressure) using ideal gas equation PV = nRT or using the molar gas volume (1mol gas =24dm^3 at room temperature and pressure

Make sure you don't leave gaps in your diagram where gas could escape



If drawing a gas syringe make sure you draw it with some measurement markings on the barrel to show measurements can be made.

Potential errors in using a gas syringe
•gas escapes before bung inserted
•syringe sticks
• some gases like carbon dioxide or sulphur dioxide are soluble in water so the true amount of gas is not measured.

Changing the Conditions of a gas

Questions may involve the same amount of gas under different conditions.

Example 15
40 cm^3 of oxygen and 60 cm^3 of carbon dioxide, each at 298 K and 100 kPa, were placed into an evacuated flask of volume 0.50 dm^3. Calculate the pressure of the gas mixture in the flask at 298 K.

There are two approaches to solving this

1. Work out amount in mol of gas using ideal gas equation then put back into ideal gas equation with new conditions
2. Or combine the equation n= PV/RT as on right

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

We can do this as the moles of gas do not change

As Temperature is the same can make the above equation $P_1V_1 = P_2V_2$

$P_2 = P_1V_1 / V_2$

$= 100000 \times 1\times 10^{-4} / 5\times10^{-4}$

$= 20\,000$Pa

Molar Gas Volume

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

Example 16 : Calculate the volume in dm^3 at room temperature and pressure of 50.0 g 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

Reacting Volumes of Gas

Equal volumes of any gases measured under the same conditions of temperature and pressure contain equal numbers of molecules (or atoms if the gas in monatomic)

Volumes of gases reacting in a balanced equation can be calculated by simple ratio

Example 17 500 cm^3 of methane is combusted at 1atm and 300K. Calculate the volume of oxygen needed to react and calculate the volume of CO_2 given off under the same conditions..

$CH_4(g)$ +	**2** $O_2(g)$ →	$CO_2(g)$ + $2\ H_2O(l)$
1 mole	**2** mole	1 mole
500cm^3	1dm^3	500cm^3

Simply multiply gas volume x2

Example 18 An important reaction which occurs in the catalytic converter of a car is:
$2CO(g) + 2NO(g) \rightarrow 2CO_2(g) + N_2(g)$
In this reaction, when 500 cm^3 of CO reacts with 500 cm^3 of NO at 650 °C and at 1 atm.
Calculate the **total** volume of gases produced at the same temperature and pressure

$2CO(g)$ +	$2NO(g)$ →	$2CO_2(g)$ +	$N_2(g)$
500cm^3	500cm^3	**500cm^3**	**250cm^3**

total volume of gases produced = 750cm^3

Avogadro's Constant

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 Constant

There are 6.02×10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.02×10^{23} of that entity':

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

1 mole of copper atoms will contain 6.02×10^{23} atoms
1 mole of carbon dioxide molecules will contain 6.02×10^{23} molecules
1 mole of sodium ions will contain 6.02×10^{23} ions

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

Example 19 : Calculate the number of atoms of tin in a 6.00 g sample of tin metal.

amount = mass/*A*r

= 6/ 118.7

= 0.05055 mol

Number atoms = amount x 6.02×10^{23}

= 0.05055 x 6.02×10^{23}

= 3.04×10^{22}

Example 20 : Calculate the number of chloride ions in a 25.0 cm^3 of a solution of magnesium chloride of concentration 0.400 mol dm^{-3}

amount= concentration x Volume
$MgCl_2$ = 0.400 x **0.025**

= 0.0100 mol

amount 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^- = amount x 6.02×10^{23}

= 0.0200 x 6.02×10^{23}

= 1.204×10^{22}

Density

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

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

Density is usually given in g cm^{-3}
Care needs to be taken if different units are used.

Example 21 : Calculate the number of molecules of ethanol 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

= 394.5 g

amount = mass/*M*r

= 394.5/ 46.0

= 8.576 mol

Number of molecules= amount x 6.022×10^{23}

= 8.576 x 6.022×10^{23}

= 5.16×10^{24}(to 3 sig fig)

Example 22: There are 980mol of pure gold in a bar measuring 10 cm by 20 cm by 50 cm. Calculate the density of gold in kg dm^{-3}

Mass = amount x *M*r

= 980 x 197

= 193060 g

= 193.06 kg

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

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

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 mol of N_2 reacts with 3 mol of H_2 to produce 2mol of NH_3

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

Step 1:
Use one of the above 3 equations to convert any given quantity into amount in mol
Mass → amount
Volume of gas → amount
Conc and vol of solution → amount

→

Step 2:
Use balanced equation to convert amount in mol of initial substance into amount in mol of second substance

→

Step 3
Convert amount, in mol, of second substance into quantity question asked for using relevant equation
e.g. amount ,Mr → mass
Amount gas → vol gas
amount, vol solution → conc

Example 23: Calculate the mass of carbon dioxide produced from heating 5.50 g of sodium hydrogencarbonate
$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$

Step 1: Calculate amount, in mol, of sodium hydrogencarbonate
amount = mass / *M*r
= 5.5 /84
= 0.0655 mol

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

Step 3: Calculate mass of CO_2
Mass = amount x *M*r
= 0.0328 x 44.0
=1.44 g

Example 24: 23.6cm^3 of H_2SO_4 neutralised 25.0cm^3 of 0.150M NaOH. Calculate the concentration of the H_2SO_4
$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$

Step 1: Calculate amount, in mol, of sodium hydroxide
amount = 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 Calculate concentration of H_2SO_4

conc= amount/volume

= 0.001875 / 0.0236

= 0.0794 mol dm^{-3}

Example 25: Calculate 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
amount= mass / *M*r
= 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 $^5/_2$) mol gas

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

Example 26: Calculate the mass of copper that reacts completely with 150 cm^3 of 1.60 mol dm^{-3} nitric acid
$3Cu + 8HNO_3 \rightarrow 3Cu(NO_3)_2 + 2NO + 4H_2O$

Step 1: work out amount, in mol, of nitric acid
amount = conc x vol
= 1.60 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: Calculate mass of Cu
Mass = amount x *M*r
= 0.09 x 63.5
=5.71 g

Limiting and excess reactants

Example 27 Calculate the maximum mass of titanium that could be produced from reacting 100 g of $TiCl_4$ with 80.0 g of sodium.

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

Step 1: Calculate 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 1$TiCl_4$: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 mol of Na which is an excess of 1.372 mol. 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: Calculate mass of Ti formed
Mass = amount x *M*r
= 0.527 x 47.9
=25.24 g

% Yield

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

% yield in a process can be lowered through incomplete reactions, side reactions, losses during transfers of substances, losses during purification stages.

Example 28: 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 the maximum mass of Fe that could be produced

Step 1: work out amount in mol of Iron oxide
amount = mass / *M*r
=25 / 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 = amount x *M*r
= 0.313 x 55.8
=17.48 g

% yield = (actual yield/theoretical yield) x 100
= (10/ 17.48) x 100
=57.2%

% Atom Economy

$$\text{percentage atom economy} = \frac{\text{mass of useful products}}{\text{mass of all reactants}} \times 100$$

Do use **balancing numbers** when calculating % atom economy.

Example 29 : Calculate the % atom economy for the following reaction where Fe is the desired product assuming the reaction goes to completion.

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

$$\%\text{ atom economy} = \frac{(2 \times 55.8)}{(2 \times 55.8 + 3\times16) + 3 \times (12+16)} \times 100$$

$=45.8\%$

Sustainable chemistry requires chemists to design processes with high atom economy that minimise production of waste products.

Reactions where there is only one product where all atoms are used making product are ideal and have 100% atom economy.
e.g. $CH_2{=}CH_2 + H_2 \rightarrow CH_3CH_3$

If a process does have a side, waste product the economics of the process can be improved by selling the bi-product for other uses