1.2 Amount of Substance

Relative masses, Mr:

- Where 1/12th of Carbon 12 is essentially the mass of a proton / neutron.
- The first 2 definitions you've come across in the last unit.
- Additional ones are added for covalent and ionic compounds

For atoms:

RAM, Relative Atomic Mass: the weighted mean mass of an atom compared with 1/12th of the mass of carbon -12

For Isotopes:

Relative isotopic mass: the mass of an isotope compared with 1/12th of the mass of carbon -12

For covalent molecules (non metal & non metal):

Relative molecular mass, Mr: the weighted mean mass of a molecule compared with 1/12th of the mass of carbon -12

For ionic compounds (metal & non metal):

Relative formula mass, Mr: the weighted mean mass of a formula unit compared with 1/12th of the mass of carbon -12

The Mole and Avogadro's constant

- Since atoms are so small and therefore have such a small mass we have to measure them in large numbers which we call a mole.
- The simplest way to understand the mole is to treat it as a word to describe a number, such as:

Dozen	Tonne	Grand	Mole
12	**100**	**1000**	**6.02×10^{23}**

- It does appear to be quite an unusual number but it was carefully thought out by **Avogadro**
- It is the number of atoms of an element to make its **atomic mass number**
- It is called **Avogadro's constant, N_A**

Avogadro's constant, N_A: 6.02×10^{23}

Basically in 12g of carbon-12 you would find 6×10^{23} atoms of carbon.

1g of ^{1}H atoms would have 6×10^{23} atoms of H
16g of ^{16}O atoms would have 6×10^{23} atoms of O (atom is 16 x heavier than H)
32g of ^{32}S atoms would have 6×10^{23} atoms of S (atom is 32 x heavier than H)

When you think about it like this it actually makes sense!!!

- In fact if you were to measure out **6×10^{23} (A Mole)** atoms of any element you would find that its mass is the same as its **Relative Atomic Mass**

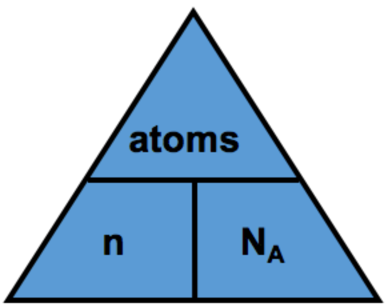
1 Mole of Sodium ^{23}Na **23**g mol^{-1}
1Mole of Magnesium ^{24}Mg **24**g mol^{-1}
1 Mole of Iron ^{56}Fe **56**g mol^{-1}

- A molecule is made up from more than 1 atom so the mass of 1 mole of that molecule will be the sum of the **Relative Atomic Masses**

1 Mole of water H_2O 18g mol^{-1}
1Mole of Sodium Chloride NaCl 58.5g mol^{-1}

Number of particles = Number of Moles x Avogadro's constant

N^{o} particles = Moles x N_A



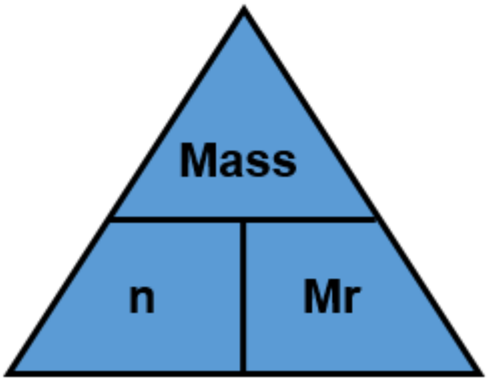
Using Moles

- There are 3 mole formulas you require depending on the units you are working in:

1) Moles and mass, (s) – grams, g

- If 1 Mole of water is 18g then 2 moles would be 36g. 3 moles would be 54g and 0.5 moles would be 9g.

Number of moles = $\frac{\text{Mass of substance}}{\text{Mr}}$	$n = \frac{m}{Mr}$



***TIP:* mass must be in g so make sure you can convert to this.**
k means 1000's of, ie 1000 of grams:

X 1000	*/ 1000*
1kg → 1000g	*1000g → 1kg*
X 1 x 10^6	*/ 1 x 10^6*
1tonne → 1000000g	*1000000g → 1tonne*

Example:

a) How many moles of water in 36g of H_2O

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

$$n = \frac{36}{18}$$

$$n = 2 \text{ moles}$$

b) What is the mass of 0.5 moles of NaCl

$$m = n \times Mr$$

$$m = 0.5 \times 58.5$$

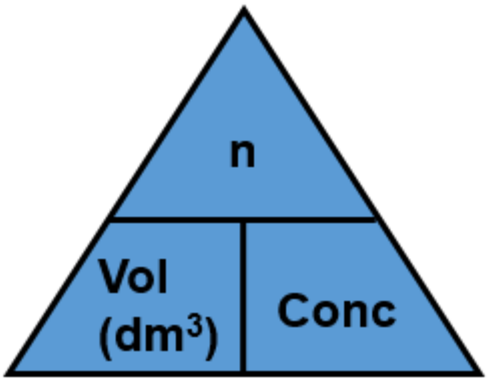
$$m = 29.25g$$

2) Moles and Solutions, (aq) – mol dm^{-3}

- A solution is expressed as a number of moles in 1dm^3 of solution .

Number of moles	=	Concentration (mol dm^{-3})	x	Volume (dm^3)

n = C x V (dm^3)

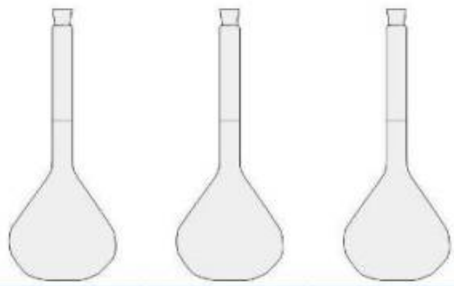


<u>TIP:</u> Volume must be in dm^3 so make sure you can convert to this:

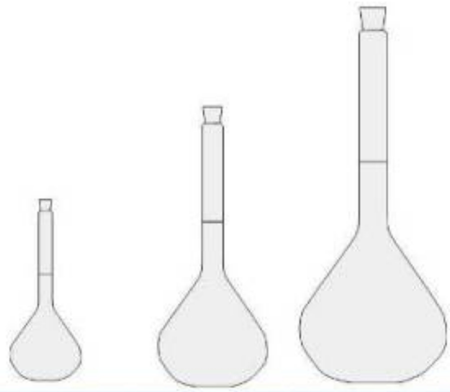
1dm^3 = 1000cm^3 = 1litre

X 1000
1dm^3 → 1000cm^3

/ 1000
1000cm^3 → 1dm^3



Volume (dm^3)	1.0 dm^3	1.0 dm^3	1.0 dm^3
Moles dissolved	2.0 mole	1.0 mole	0.5 mole
Concentration	2.0 mol dm^{-3}	1.0 mol dm^{-3}	0.5 mol dm^{-3}
Calculated by	Moles / Vol (dm^3)	Moles / Vol (dm^3)	Moles / Vol (dm^3)
	2.0 / 0.5	1.0 / 1.0	1.0 / 2.0



Volume (dm^3)	0.5 dm^3	1.0 dm^3	2.0 dm^3
Moles dissolved	1.0 mole	1.0 mole	1.0 mole
Concentration	2.0 mol dm^{-3}	1.0 mol dm^{-3}	0.5 mol dm^{-3}
Calculated by	Moles / Vol (dm^3)	Moles / Vol (dm^3)	Moles / Vol (dm^3)
	2.0 / 0.5	1.0 / 1.0	1.0 / 2.0

Example:

Calculate the number of moles of NaOH in 50cm^3 of a 0.30 Mol dm^{-3} solution

n = C x V (dm^3)   V is in dm^3 50/1000 = 0.05

n = 0.3 x 0.05

n = 0.015 moles

Standard solutions calculations

- These are calculations to make a smaller volume of a specific concentration
- These combine both of the mole formulas in a calculation:

$$\textbf{Number of moles} = \frac{\textbf{Mass of substance}}{\textbf{Mr}}$$

$$\textbf{Number of moles} = \textbf{Concentration} \times \textbf{Volume}$$

Example:

What mass of NaOH is required to make $250cm^3$ of 0.1 mol dm^{-3} solution of sodium hydroxide?

- To calculate the mass, we need moles
- So, we have to calculate the moles from volume and concentration first:

n = C x V (dm^3) V is in dm^3 250/1000 = 0.25

n = 0.1 x 0.25

n = 0.025 moles

- Now calculate the mass from moles

m = n x Mr

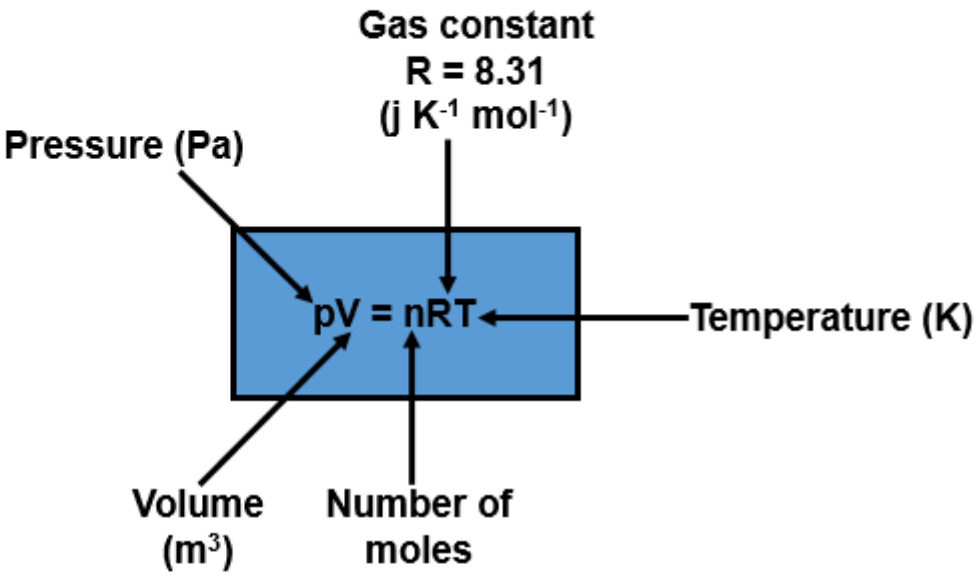
m = 0.025 x 40

m = 1.00g

3) Moles and gases, (g) – M^3

- The volume of a gas can vary depending on **temperature** and **pressure**.
- These need to be taken into account when dealing with **moles** and **gases**

The Ideal gas equation



2 assumptions:

- The volume of the molecules is negligible
- The molecules have no intermolecular forces of attraction

TIP: ***Volume must be in m^3 so make sure you can convert to this:***

$$1000000cm^3 = 1000dm^3 = 1m^3$$

$1m^3 \xrightarrow{\times 1000} 1000dm^3$	$1000dm^3 \xrightarrow{\times 1000} 1000000cm^3$	$1m^3 \xrightarrow{\times 1000000} 1000000cm^3$
$1000000cm^3 \xrightarrow{/1000} 1000dm^3$	$1000dm^3 \xrightarrow{/1000} 1m^3$	$1000000cm^3 \xrightarrow{/1000000} 1m^3$

TIP: ***Temperature must be in kelvin, K so make sure you can convert to this:***

$0^oC \xrightarrow{+273} 273K$	$100^oC \xrightarrow{+273} 373K$	$25^oC \xrightarrow{+273} 298K$
$273K \xrightarrow{-273} 0^oC$	$373K \xrightarrow{-273} 100^oC$	$298K \xrightarrow{-273} 25^oC$

Examples:

a) How many moles are there in $0.05m^3$ of Nitrogen gas, at 273K and 100000Pa

P V = n R T Rearrange to get n on its own, divide both sides by RT

$$n = \frac{P\,V}{R\,T}$$

$$n = \frac{100000 \times 0.05}{8.31 \times 273}$$

n = 2.20 moles

b) What is the volume occupied when 4 moles of Chlorine gas is at 27^oC and 100 kPa?

Convert units to SI units first:

T = 27 + 273 = 300K **P = 100 x 1000 = 100000Pa**

P V = n R T Rearrange to get V on its own, divide both sides by p

$$V = \frac{n\,R\,T}{P}$$

$$V = \frac{4 \times 8.31 \times 300}{100000}$$

V = 0.0997 m^3

c) What mass of oxygen gas, O_2 that has a volume of $1200cm^3$ at 25^oC and 200 kPa?

To get mass, we need moles and Mr. We have to use PV = nRT first to get moles, n

Convert units to SI units first:

T = 25 + 273 = 298K **P = 200 x 1000 = 200000Pa** **V = 1200 / 1000000 = 0.0012m^3**

P V = n R T Rearrange to get n on its own, divide both sides by RT

$$n = \frac{P\,V}{R\,T}$$

$$n = \frac{200000 \times 0.0012}{8.31 \times 298}$$

n = 0.0969 moles Now use the moles in the mass equation

mass = n x Mr

mass = 0.0969 x 32

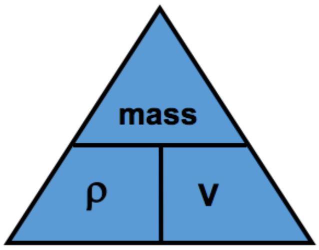
mass = 3.10g

Density

Density, ρ: is the amount of substance (g) per unit volume (cm^3)

- The whole density scale is measured against water which has a density of 1 gcm^{-3}
- This means that in 1cm^3 of water there is 1g of water

The equation:



- The mass, volume and density could be in any combination of mass or volume units so make sure your units are consistent in the question

Example calculations:

1) Calculate the density of ethanol in g cm^{-3} given a mass of 19g in a volume of 25cm^3?

$$\rho = m / V$$

$$\rho = 19 / 25$$

$$\rho = 0.76 \text{ g cm}^{-3}$$

2) Calculate the density of gold in g cm^{-3} given that a gold bar contains 5 moles of gold and is 5.3cm wide, 11.8cm long and 0.8cm thick?

$m = n \times Mr$

$m = 5 \times 197$

$m = 1000g$

$V = 5.3 \times 11.8 \times 0.8$

$V = 50 \text{ cm}^3$

$$\rho = m / V$$

$$\rho = 1000 / 50$$

$$\rho = 20 \text{ g cm}^{-3}$$

Empirical and Molecular formula

***Empirical formula**: is the simplest whole number ratio of atoms of elements in a molecule*

***Molecular formula**: is the actual number ratio of atoms of elements in a molecule*

Examples:

a) A sample of iron oxide was found to have 11.2g of iron and 4.8g of oxygen. Calculate the formula of this compound

Element	**Fe**		**O**
Masses	**11.2**		**4.8**
Divide by Ar	**11.2 / 55.8**		**4.8 / 16**
Moles	**0.2**	**:**	**0.3**
Divide by smallest	**0.2 / 0.2**	**:**	**0.3 / 0.2**
Ratio	**1**	**:**	**1.5**
Whole No Ratio	**2**	**:**	**3**
Empirical formula	**Fe_2O_3**		

b) A sample of hydrocarbon was found to have 1.20g of carbon and 0.25g of hydrogen. Calculate the Empirical formula of this compound. Then find out the molecular formula if the Mr = 58

Element	**C**		**H**
Masses	**1.20**		**0.25**
Divide by Ar	**1.20 / 12**		**0.25 / 1**
Moles	**0.10**	**:**	**0.25**
Divide by smallest	**0.10 / 0.10**	**:**	**2.5 / 0.10**
Ratio	**1**	**:**	**2.5**
Whole No Ratio	**2**	**:**	**5**
Empirical formula	**C_2H_5 (29 x 2 = 58)**		
Molecular formula	**C_4H_{10}**		

TIP:
%'s may be used instead of masses, treat the calculation in the same way as %'s, these could be thought of as masses in 100g

You may have to calculate the mass or % of an element in a sample by taking the mass of one element from the total mass of the compound

Moles and reactions

- Mole calculations can now be used to calculate reacting amounts / product amounts.
- This is done by using the balanced chemical equation and moles calculations using masses, gas volumes and concentrations.
- **ALL 3** of these require the use of the mole:

A) Mass / mole calculations:

Example: 7.82g of potassium reacts in air to form potassium oxide. Calculate the mass of potassium oxide made:

STEP1: Write a balanced chemical equation and add the amounts given and question mark what you are asked to work out:

$$2K_{(s)} + \tfrac{1}{2}O_{2(g)} \rightarrow K_2O_{(s)}$$

7.82g — m = ?

STEP2: Check the state symbol of your starting mass to decide which moles equation you will use - **(s) - means you use Moles = mass / Ar**

$$2K_{(s)} + \tfrac{1}{2}O_{2(g)} \rightarrow K_2O_{(s)}$$

7.82g — m = ?

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

$n = 7.82 / 39.1$

$n = 0.2$

STEP3: Use the reacting **ratios** to work out how many moles you have made (or need):

$$2K_{(s)} + \tfrac{1}{2}O_{2(g)} \rightarrow K_2O_{(s)}$$

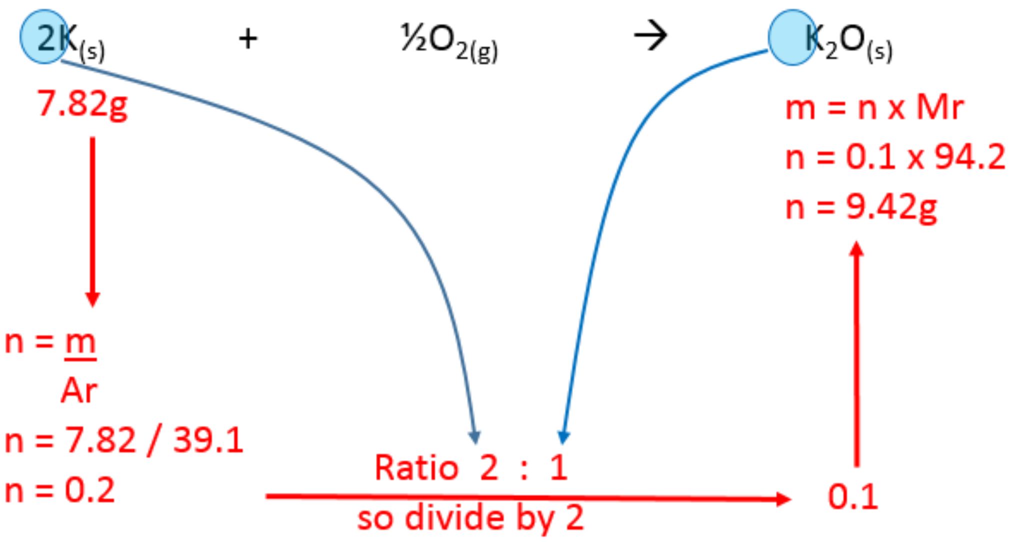
7.82g — m = ?

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

$n = 7.82 / 39.1$

$n = 0.2$ $\xrightarrow[\text{so divide by 2}]{\text{Ratio } 2 : 1}$ 0.1

STEP4: Check the question/ state symbol to decide whether to convert it to mass / concentration / volume - (s) = mass



- These are usually done as a series of steps but the process is the same:

$$2K_{(s)} \quad + \quad ½O_{2(g)} \quad \rightarrow \quad K_2O_{(s)}$$

7.82g m = ?

Calculate moles of potassium

n of K = mass / Ar

n of K = 7.82 / 39.1

n of K = 0.2

Calculate moles of potassium oxide

n of K_2O = 0.2 / 2 (ratio 2:1, divide by 2)

n of K_2O = 0.1

Calculate mass of potassium oxide

mass of K_2O = n x Mr

mass of K_2O = 0.1 x 94.2

mass of K_2O = 9.42g

B) Gas / mole calculations:

Example: 1.15g sodium reacts with excess sulphuric acid to form sodium sulphate and hydrogen gas.
Calculate the volume of hydrogen made in m^3 if the reaction was carried out at 25°C and 100 kPa:

STEP1: Write a balanced chemical equation and add the amounts given and question mark what you are asked to work out:

$$2Na_{(s)} \quad + \quad H_2SO_{4(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_{2(g)}$$

1.15g V=?

STEP2: Check the state symbol of your starting mass to decide which moles equation you will use - **(s) - means you use Moles = mass / Ar**

$$2Na_{(s)} \quad + \quad H_2SO_{4(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_{2(g)}$$

1.15g V=?

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

n = 1.15 / 23.0

n = 0.05

STEP3: Use the reacting **ratios** to work out how many moles you have made (or need):

$$2Na_{(s)} \quad + \quad H_2SO_{4(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_{2(g)}$$

1.15g V=?

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

n = 1.15 / 23.0

$$n = 0.05 \xrightarrow[\text{so divide by 2}]{\text{Ratio } 2 : 1} 0.025$$

STEP4: Check the question/ state symbol to decide whether to convert it to mass / concentration / volume - (g) = volume

$$2Na_{(s)} \quad + \quad H_2SO_{4(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_{2(g)}$$

1.15g

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

n = 1.15 / 23.0

n = 0.05

Ratio 2 : 1

so divide by 2

0.025

$$V = \frac{nRT}{P}$$

$$V = \frac{0.025 \times 8.31 \times 298}{100000}$$

$$V = 6.19 \times 10^{-4}\ m^3$$

- Again, these can be done as a series of steps:

$$2Na_{(s)} \quad + \quad H_2SO_{4(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_{2(l)}$$

1.15g V=?

Calculate moles of sodium

n of Na = mass / Ar

n of Na = 1.15 / 23

n of Na = 0.05

Calculate moles of hydrogen

n of H_2 = 0.05 / 2 (ratio 2:1, divide by 2)

n of H_2 = 0.025

Calculate volume of H_2

Vol of H_2 = nRT / P

Vol of H_2 = 0.025 x 8.31 x 298 / 100000

Vol of H_2 = $6.19 \times 10^{-4}\ m^3$

Required Practical 1 - Titrations

- This technique can be used to find:

Concentration **Mr** **Formula** **Water of crystalisation**

- To do this you react a certain volume of a solution with an unknown concentration with a solution of **known concentration**.
- The concentration of the known solution must be accurate and is known as a **standard solution.**

Making a standard solution – Making 250cm^3 of a 0.1 mol dm^{-3} solution of NaOH

- Weigh a known mass (number of moles) out in a weighing boat recording its mass to the number of decimal places on the balance.

n = C x V (dm^3) (250/1000 = 0.25)

n = 0.1 x 0.25

n = 0.025 moles

m = n x Mr

m = 0.025 x 40

m = 1.00g

- Transfer to a beaker and reweigh the weighing boat (as there may be some left in the weighing boat). The difference is the **precise** mass added to a beaker:

Mass of weighing boat + calculated mass NaOH	2.62g
Mass of weighing boat	1.63g
Mass of NaOH dissolved	**0.99g**

- Dissolve in 100cm^3 of distilled water and stir with a glass rod.
- Using a funnel, pour into a volumetric flask.
- Use the wash bottle to wash beaker, funnel and glass rod into the volumetric flask.
- Fill the volumetric flask with distilled water so the meniscus sits on the line.
- Stopper the flask and invert several times to ensure mixing.
- Now calculate the **exact concentration**:

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

$n = \frac{0.99}{40}$

n = 0.02475 moles

$C = \frac{n}{V}$

$C = \frac{0.02475}{0.25}$

C = 0.099 mol dm^{-3}

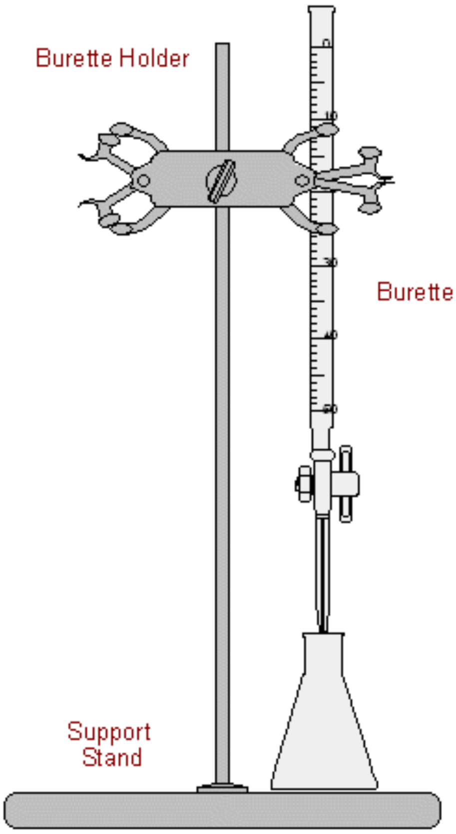
Carrying out a titration:

- Using moles and reacting ratios, you can calculate the concentration of a solution.
- The unknown goes in the conical flask and the known goes in the burette
- The only requirement is that you can tell when one solution has completely reacted with the other.
- Between acids and alkalis, we use indicators to let us know when the resulting solution is neutral.
- An indicator will change colour at the 'end point' (neutral).
- Common indicators are:

Indicator	Acidic colour	Base colour	End point colour
Methyl orange	Red	Yellow	Orange
Phenylphthalein	colourless	Pink	Pale pink

Technique/procedure

Example – finding an unknown concentration of NaOH using 0.10 moldm^{-3} H_2SO_4



1) Rinse the burette with sulphuric acid, H_2SO_4.
2) Fill the burette to the graduation mark ensuring the air is removed from the tap.
3) Rinse a pipette with sodium hydroxide, NaOH fill and transfer 25 cm^3 to a clean, dry conical flask.
4) Add 2-3 drops of indicator.
5) Run the acid into the alkali and stop when the colour changes. This is your **'trial'**.
6) Record the burette readings to 2dp ending 0 / 5
7) Repeat the titration until you get **2 concordant results**
8) Calculate the mean titre to 2dp.

Record results in a table like the one below:

	Trial	1	2	3
Final burette reading /cm^3				
Initial burette reading /cm^3				
Titre /cm^3				
Mean Titre 2dp /cm^3				

C) Aqueous solution / mole calculation – example

In a titration 0.01M sulphuric acid was added to 25cm^3 of sodium hydroxide. Calculate the concentration of the sodium hydroxide given the following results:

	Trial	1	2
Final burette reading /cm^3	**22.3**	**21.8**	**21.7**
Initial burette reading /cm^3	**0.00**	**0.00**	**0.00**
Titre /cm^3	**22.3**	**21.8**	**21.7**
Mean Titre 2dp /cm^3		**21.75**	

1 Write a balanced equation

$$H_2SO_{4(aq)} \quad + \quad 2NaOH_{(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_2O_{(l)}$$

2 Calculate the number of moles of acid added from the burette

$$H_2SO_{4(aq)} \quad + \quad 2NaOH_{(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_2O_{(l)}$$

C = 0.01 moldm^{-3}
V = (21.75cm^3)
21.75 x 10^{-3} dm^3

$\downarrow$

n = C x V
n = 0.01 x 0.02175
n = 2.175 x 10^{-4} moles

3 Use the ratio to work out the number of moles in the sample of alkali

$$H_2SO_{4(aq)} \quad + \quad 2NaOH_{(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_2O_{(l)}$$

C = 0.01 moldm^{-3}
V = (21.75cm^3)
21.75 x 10^{-3} dm^3

$\downarrow$

n = C x V
n = 0.01 x 0.02175
n = 2.175 x 10^{-4} moles $\xrightarrow[\text{x 2}]{\text{Ratio 1 : 2}}$ **4.35 x 10^{-4}**

4 Calculate the concentration.

$$H_2SO_{4(aq)} \quad + \quad 2NaOH_{(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_2O_{(l)}$$

$C = 0.01\ moldm^{-3}$
$V = (21.75cm^3)$
$21.75 \times 10^{-3}\ dm^3$

$V = (25cm^3)\ \ 0.025dm^3$

$C = \dfrac{4.35 \times 10^{-4}}{0.025}$

$\underline{\mathbf{C = 0.0174\ moldm^{-3}}}$

$n = C \times V$
$n = 0.01 \times 0.02175$
$\mathbf{n = 2.175 \times 10^{-4}\ moles} \xrightarrow[\times 2]{\text{Ratio } 1 : 2} \mathbf{4.35 \times 10^{-4}}$

- Again, these can be done as a series of steps:

1 Write a balanced equation

$$H_2SO_{4(aq)} \quad + \quad 2NaOH_{(aq)} \quad \rightarrow \quad Na_2SO_{4(aq)} \quad + \quad H_2O_{(l)}$$

2 Calculate the number of moles of H_2SO_4 added from the burette

n of H_2SO_4 = C x V

n of H_2SO_4 = 0.01 x 0.02175

n of H_2SO_4 = 2.175 x 10^{-4}

3 Use the ratio to work out the number of moles of NaOH in the conical flask

H_2SO_4 : NaOH 1 : 2

n of NaOH = 2.175 x 10^{-4} x 2

n of NaOH = 4.35 x 10^{-4}

4 Calculate the concentration of NaOH

$C = \dfrac{4.35 \times 10^{-4}}{0.025}$

C = 0.0174 $moldm^{-3}$

TIP:
Mass, gas and aqueous solution formulas may be used in a combination of ways in these reacting mole calculations

The format remains the same – a starting point – an end point, in the balanced equation

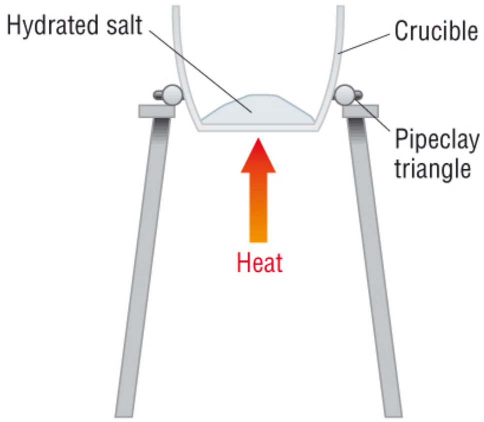
Water of crystallisation

- Coloured crystals such as blue copper sulphate have water molecules attached to the ions.
- The water can be driven by heat, leaving white copper sulphate crystals.
- This water locked in the crystal is called the **water of crystallisation**.

Hydrated - Crystals that contain water

Anhydrous - Crystals that do not contain water

- The water can be evaporated by heat. Some compounds will decompose so a moderate heat must be used:



- The waters in the crystal obviously have a mass and will affect the Mr of the crystal.
- The water must be written in the formula. This is done by following a dot after the crystal formula:

$CuSO_4.5H_2O$

- For copper sulphate, 1 mole of copper sulphate crystals will contain 5 moles of water:
- The number of moles of water per mole of crystal depends upon that crystal:

$CuSO_4.5H_2O$
$CoCl_2.6H_2O$

From mole calculations (example)

Mass of hydrated $MgSO_4.xH_2O$ = 4.312g
Mass of anhydrous $MgSO_4$ = 2.107g

	Crystal, $MgSO_4$	**Water, H_2O**
Masses of each	2.107g	(4.312 - 2.107)
	2.107g	**2.205g**
Moles of each	2.107 / 120.4	2.205 / 18
	0.0175	**0.1225**
Divide by the smallest	0.0175 / 0.0175	0.1225 / 0.0175
	1	**7**

So the formula of hydrated $MgSO_4.xH_2O$ = $MgSO_4.7H_2O$

Percentage yield:

Is a measure of how wasteful a chemical process is

- When we think about reactions, we always think of them as going 100% to products.
- This is usually **not** the case due to:

Equilibria **Side reactions** **Purity** **Transfers** **Separation / purification**

- Percentage yield is like a score in a test. It is an indication of what you achieved out of what you could have got:

$$\textbf{\% Yield} = \frac{\textbf{Actual yield}}{\textbf{Theoretical yield}} \times 100$$

The rules:

1. **Write a balanced chemical equation**
2. **Calculate the theoretical amount of product in moles**
3. **Calculate the theoretical amount of product in g**
4. **Calculate % yield using the formula:**

$$\textbf{\% Yield} = \frac{\textbf{Actual Yield}}{\textbf{Theoretical Yield}} \times 100$$

Examples:

A) Preparation of ethanoic acid:
A student reacted 9.20g of ethanol with and excess of sulphuric acid and sodium dichromate (the oxidising agent). The student obtained 4.35g of ethanoic acid. Calculate the % yield:

1) Write a balanced chemical equation:

$$CH_3CH_2OH + 2[O] \rightarrow CH_3COOH + H_2O$$

2) Calculate the theoretical amount of moles of product:

- Calculate the amount of moles of ethanoic acid you could have made:

CH_3CH_2OH	+	2[O]	→	CH_3COOH	+	H_2O
9.20g				**Actual Yield = 4.35g**		
↓						

Moles =	mass / Mr				
Moles =	9.20 / 46.0	**1:1**			
Moles =	0.200 moles		→	Theoretical Moles	0.200 moles

3) Calculate the theoretical amount of product obtained in g:

- Calculate the number of moles you actually made:
- Calculate the amount of moles of ethanoic acid you could have made:

CH_3CH_2OH	+	2[O]	→	CH_3COOH	+	H_2O
9.20g				**Actual Yield = 4.35g**		
↓				**Theoretical Yield = 12.00g**		
Moles = mass / Mr				**Theoretical mass = 0.2 x 60**		
Moles = 9.20 / 46.0			**1:1**	↑		
Moles = 0.200 moles			→	Theoretical Moles	0.200 moles	

5) Calculate % yield using the formula:

$$\text{\% Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

$$= \frac{4.35}{12.00} \times 100$$

$$= \mathbf{36.25\%}$$

<u>Atom economy:</u>

Is a measure of how wasteful a reaction is

- Atom economy takes into account any wasteful by products too
- By products are considered wasteful as they are usually disposed of. This is costly and can cause environmental problems.
- A more efficient way of dealing with by products would be to sell them on to companies that would make use of them.

$$\textbf{Atom economy} = \frac{\text{Mr of the desired product}}{\text{Sum of Mr's of all products}} \times 100$$

Atom economy – Type of reaction:

- Reactions having only one product have a high atom economy. The type of reactions giving only one product are **addition reactions**.
- Reactions giving more than one product have a low atom economy. The type of reactions giving more than one product are **substitution / elimination reactions**.
- To improve the atom economy for **substitution / elimination** reactions, a use for the undesired product should be found.
- If the undesired product is toxic, we have even bigger problems -disposal.

Atom economy – Economic advantage

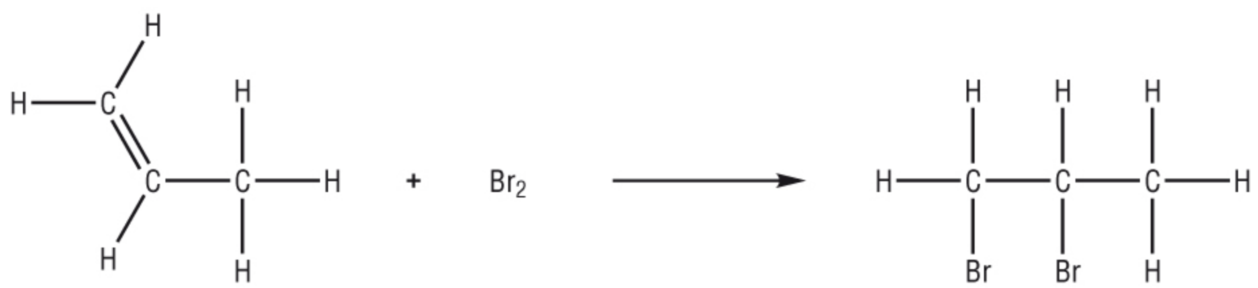
- Reactions that use a lot of starting materials to make a small amount of product has high waste.
- Reactions that give many other products apart from the desired products has high waste.
- Both of these will cost more money to make.
- Reducing the waste reduces cost – eg Ibuprofen has improved from 40% → 77%.

Atom Economy – Environment / ethics

- Raw materials – usually have limited supply so using them more efficiently makes them last longer.
- Waste materials – Disposal can be problematic as chemical waste is often harmful.
- Reducing both of the above 2 points can:
  - Reduce the demand on the worlds resources
  - Reduce the cost making them cheaper and more available

Calculating atom economy:

A) Bromination of propene:



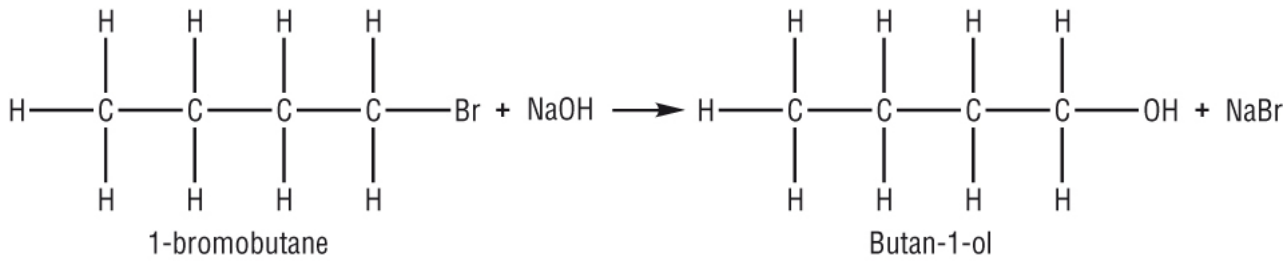
$$\text{Atom economy} = \frac{\text{Mr of the desired product}}{\text{Sum of Mr's of all products}} \times 100$$

$$= \frac{201.8}{201.8} \times 100$$

$$= 100\%$$

- Any reaction that gives only one product is very atom economic, addition reactions for example.

B) Preparation of butan - 1 - ol:



$$\text{Atom economy} = \frac{\text{Mr of the desired product}}{\text{Sum of Mr's of all products}} \times 100$$

$$= \frac{74.0}{176.9} \times 100$$

$$= 41.8\%$$

- This means that most of the starting materials ended up as waste.