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 <u>Atomic</u> Mass: the weighted mean mass of an <u>atom</u> compared with 1/12th of the mass of carbon -12

For Isotopes:

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

For covalent molecules (non metal & non metal):

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

For ionic compounds (metal & non metal):

Relative <u>formula</u> mass, Mr: the weighted mean mass of a <u>formula unit</u> 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 x 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 X 10^{23}

Basically in 12g of carbon-12 you would find 6x10^{23} atoms of carbon.

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

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

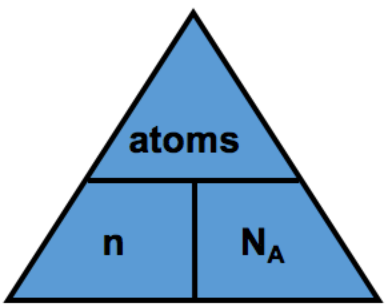
- In fact if you were to measure out **6x10^{23} (A Mole)** atoms of any element you would find that its mass is the same as its **Relative Atomic Mass**

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

Nº particles = Moles x N_A



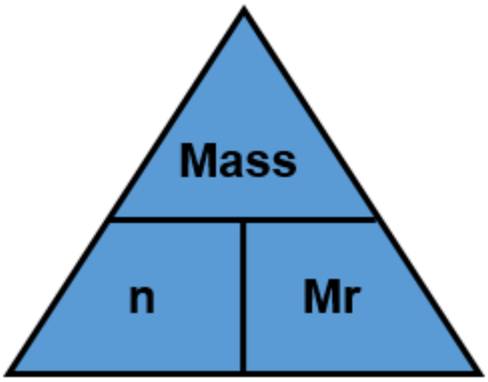
Using Moles

- 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 = $\dfrac{\text{Mass of substance}}{\text{Mr}}$	$n = \dfrac{m}{Mr}$



TIP: ***mass must be in g so make sure you can convert to this.***
k means 1000's of, ie 1000 of grams:
m means 1000th's of a gram, 0.001g

$$1000\text{ mg} \xrightarrow[\times 10^{-3}]{/1000} 1\text{ g} \xrightarrow[\times 10^{-3}]{/1000} 0.001\text{ kg} \xrightarrow[\times 10^{-3}]{/1000} 0.000001\text{ Tonne}$$

$$0.000001\text{ Tonne} \xrightarrow[\times 10^{3}]{\times 1000} 0.001\text{ kg} \xrightarrow[\times 10^{3}]{\times 1000} 1\text{ g} \xrightarrow[\times 10^{3}]{\times 1000} 1000\text{ mg}$$

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

$$m = n \times Mr$$

$$m = 0.5 \times 58.5$$

$$m = 29.25\text{g}$$

Questions:

1) Calculate the number of moles of 3.45g of Lithium

2) Calculate the number of moles of 243mg of Magnesium

3) Calculate the number of moles of 2.79Kg of Iron

Numbers of particles and masses

4) Calculate the number atoms of Calcium in 4.01g

5) Calculate the number atoms of sodium in 575mg

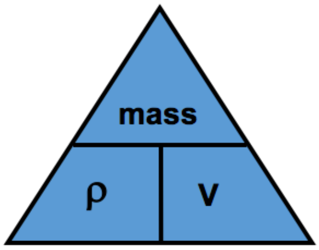
6) Calculate the number atoms of Silicon in 5.62Kg

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
- It is usually used for organic liquids (not solutions, later).

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?

$m = n \times Mr$

$m = 5 \times 197$

$m = 1000\text{g}$

$V = 5.3 \times 11.8 \times 0.8$

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

$$\rho = m / V$$

$$\rho = 1000 / 50$$

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

Questions

1) Calculate the number of moles of $5cm^3$ of Bromine, Br_2 if its density is $1.35\ gcm^{-3}$

2) Calculate the number of moles of $2cm^3$ of Ammonia, NH_3 if its density is $1.12\ gcm^{-3}$

3) Calculate the number of moles of $12cm^3$ of Hydrogen fluoride, HF if its density is $1.11\ gcm^{-3}$

4) Calculate the number of molecules in $2cm^3$ of water, H_2O if its density is $1.00\ gcm^{-3}$

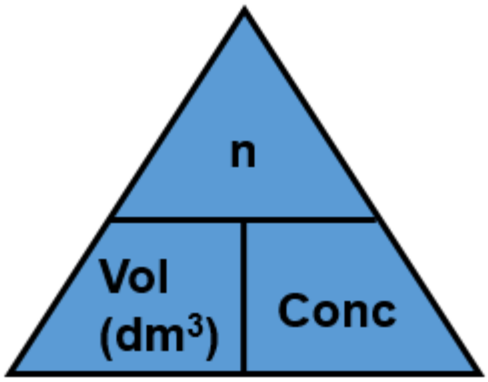
5) Calculate the number of atoms in $6cm^3$ of Mercury, Hg if its density is $3.15\ gcm^{-3}$

6) Calculate the number of atoms in $35cm^3$ of Neon, Ne if its density is $0.31\ gcm^{-3}$

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

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

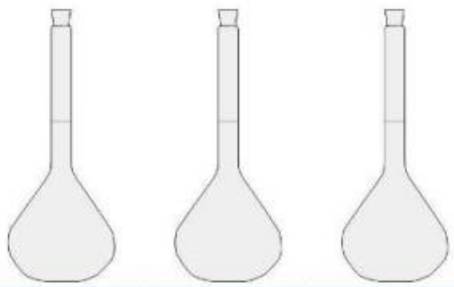
Number of moles = Concentration x Volume	**n = C x V (dm^3)**
(mol dm^{-3}) (dm^3)	



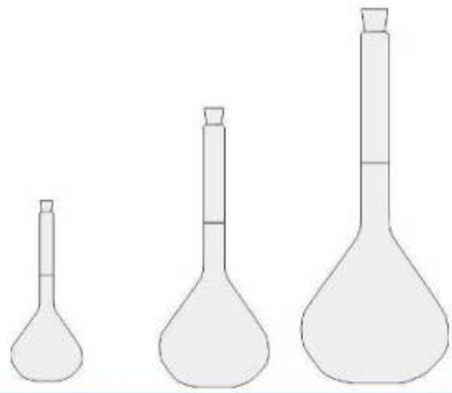
***TIP:* Volume must be in dm^3 so make sure you can convert to this:**

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

X 1000	***/ 1000***
1dm^3 → 1000cm^3	***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:

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

Number of moles = Concentration x 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

Questions

1) Calculate the number of moles in the following.

a) 2 dm^3 of 0.05 mol dm^{-3} HCl

b) 50 cm^3 of 5 mol dm^{-3} H_2SO_4

c) 10 cm^3 of 0.25 mol dm^{-3} KOH

2) Calculate the concentration of the following in **both** mol dm^{-3} and g dm^{-3}

a) 0.400 moles of HCl in 2.00 dm^3 of solution

b) 12.5 moles of H_2SO_4 in 5.00 dm^3 of solution

c) 1.05 g of NaOH in 500 cm^3 of solution

3) Calculate the volume of each solution that contains the following number of moles.

a) 0.00500 moles of NaOH from 0.100 mol dm^{-3} solution

b) 1.00×10^{-5} moles of HCl from 0.0100 mol dm^{-3} solution

4) Calculate the concentration if 561mg of KOH was dissolves in 50cm^3 of water

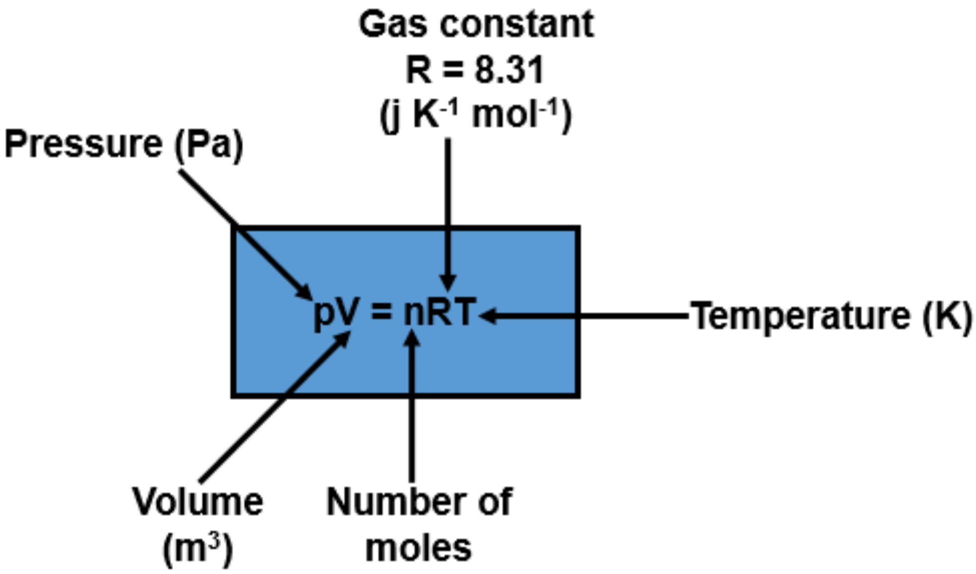
5) Calculate the concentration if 583mg of $Mg(OH)_2$ was dissolves in 25cm^3 of water

6) Calculate the concentration if 0.0126g of HNO_3 was dissolves in 100cm^3 of water

1) 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:***

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

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

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

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

Questions

1) Calculate the number of moles of a gas that occupies $10m^3$ at 373K and 100000Pa of pressure

2) Calculate the number of moles of a gas that occupies $150dm^3$ at 100^oC and 250KPa of pressure

3) Calculate the number of moles of a gas that occupies $250cm^3$ at 250^oC and 25KPa of pressure

4) Calculate the mass of N_2 gas that occupies $500cm^3$ at 350^oC and 150KPa of pressure

5) Calculate the mass of NH_3 gas that occupies $2dm^3$ at 400^oC and 350KPa of pressure

6) a) Calculate the density in gcm^{-3} of carbon dioxide gas at $25^{o}C$ at 101.325KPa

b) The Density of air is 0.997 gcm^{-3}. State whether carbon dioxide would sink or float in an enclosed room.

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:

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

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**

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

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):

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

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

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

7.82g

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

$n = 7.82 / 39.1$

$n = 0.2$

Ratio 2 : 1

so divide by 2

0.1

$m = n \times Mr$

$n = 0.1 \times 94.2$

$n = 9.42g$

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

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

7.82g $\qquad$ 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

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

$n = 1.15 / 23.0$

$n = 0.05$

Ratio 2 : 1

so divide by 2

0.025

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

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

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

- 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.

$n = C \times V (dm^3)$ (250/1000 = 0.25) $m = n \times Mr$

$n = 0.1 \times 0.25$ $m = 0.025 \times 40$

$n = 0.025$ moles **$m = 1.00g$**

- 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**:

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

$n = \frac{0.99}{40}$ $C = \frac{0.02475}{0.25}$

$n = 0.02475$ moles **$C = 0.099$ mol dm^{-3}**

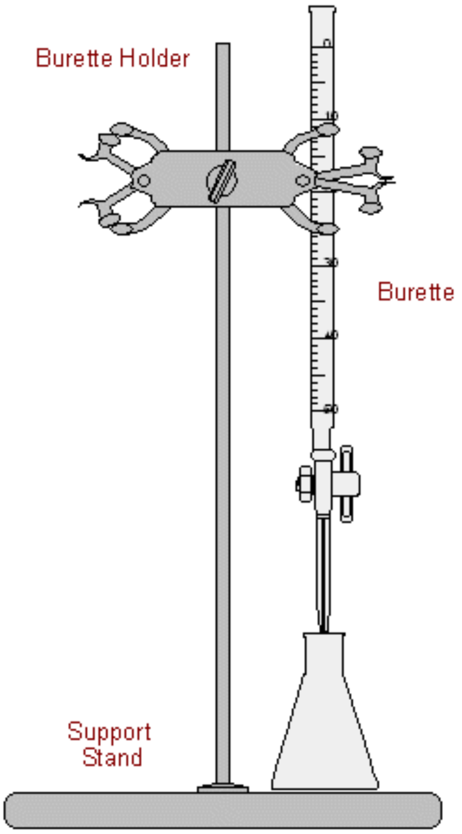
Carrying out a titration:

- 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

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

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

$\downarrow$

$n = C \times V$
$n = 0.01 \times 0.02175$
$n = 2.175 \times 10^{-4}$ moles

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

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

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

$\downarrow$

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

4 Calculate the concentration.

$H_2SO_{4(aq)}$ + $2NaOH_{(aq)}$ → $Na_2SO_{4(aq)}$ + $H_2O_{(l)}$

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

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

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

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

$n = C \times V$
$n = 0.01 \times 0.02175$

$n = 2.175 \times 10^{-4}$ moles $\xrightarrow[\times 2]{\text{Ratio } 1:2}$ **4.35×10^{-4}**

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

1 Write a balanced equation

$H_2SO_{4(aq)}$ + $2NaOH_{(aq)}$ → $Na_2SO_{4(aq)}$ + $H_2O_{(l)}$

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 = 2.175×10^{-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 = $2.175 \times 10^{-4} \times 2$

n of NaOH = 4.35×10^{-4}

4 Calculate the concentration of NaOH

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

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

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

Questions

1) 25.0 cm^3 of a solution of sodium hydroxide solution required 21.5 cm^3 of 0.100 $moldm^{-3}$ sulphuric acid for neutralisation. Find the concentration of the sodium hydroxide solution.

$H_2SO_4(aq) + 2\ NaOH(aq) \rightarrow Na_2SO_4(aq) + 2\ H_2O(l)$

2) Find the volume of 1.0 $moldm^{-3}$ hydrochloric acid that reacts with 25 cm^3 of 1.50 $moldm^{-3}$ sodium hydroxide.

$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$

3) 25.0 cm^3 of 0.100 $moldm^{-3}$ sodium hydroxide neutralises 19.0 cm^3 of hydrochloric acid. Find the concentration of the acid.

$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$

4) What volume of 0.040 $moldm^{-3}$ calcium hydroxide solution just neutralises 25.0 cm^3 of 0.100 $moldm^{-3}$ nitric acid?

$Ca(OH)_2(aq) + 2\ HNO_3(aq) \rightarrow Ca(NO_3)_2(aq) + 2\ H_2O(l)$

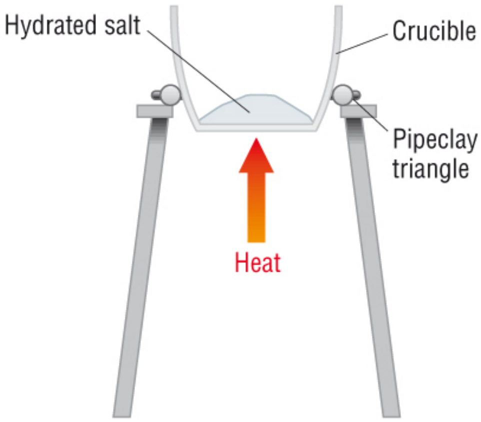
Water of crystallisation

- 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:

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

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

$$= 36.25\%$$

<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.

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

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

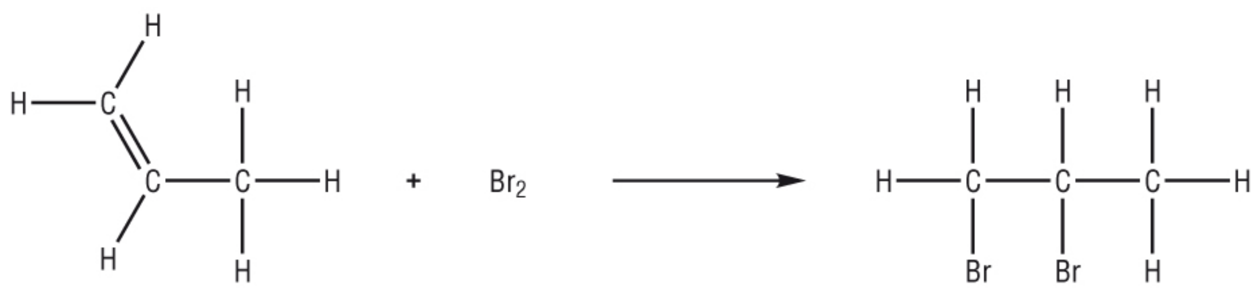
- Reactions that use a lot of starting materials to make a small amount of product has high waste.
- Reactions that give many other products apart from the desired products has high waste.
- Both of these will cost more money to make.
- Reducing the waste reduces cost – eg Ibuprofen has improved from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



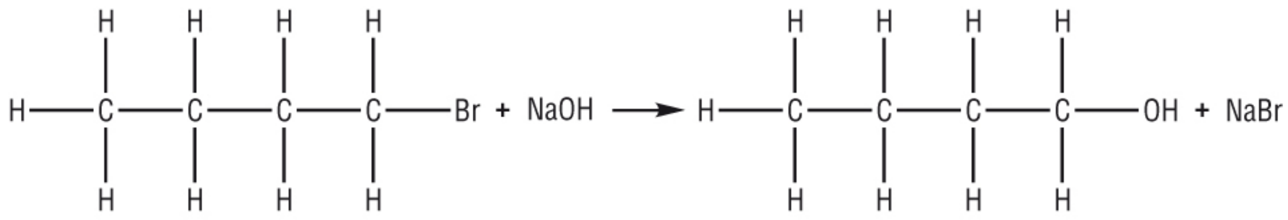
$$\textbf{Atom economy} = \frac{\text{Mr of the desired product}}{\text{Sum of Mr's of all products}} \times 100$$

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

$$= 100\%$$

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

B) Preparation of butan - 1 - ol:



1-bromobutane 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.