Chemistry Knowledge Organiser
C4 - Chemical calculations

Relative formula mass (M_r):

This is the mass in grams of 1 mole of the substance. To calculate it you need to add up the atomic mass (bigger number) of all of the atoms in the molecule.

e.g 1. NaCl = Na + Cl = 23 + 35.5 = 58.5

e.g 2. $MgF_2 = Mg + (2 \times F) = 24 + (2 \times 19) = 62$

The Mole

A mole of an element is simply **6.02×10^{23} atoms (this number is known as Avogadro's number)**. Obviously, if the atoms are larger then 1 mole of that atom will be heavier. For example, one mole of hydrogen atoms weighs 1 gram but 1 mole of carbon weighs 12 grams. To calculate the number of moles in an element you need to divide the mass by the relative atomic mass:
For example, how many moles are there in 6 grams of carbon?
6/12= 0.5

To work out the number of moles in a compound you divide the mass of the compound by the relative formula mass, for example how many moles in 30 grams of magnesium oxide (MgO)?
M_r of MgO=24+16= 40
Moles= 30/40=0.75 **Moles**

HT: Calculating Masses in Reactions

An understanding of the mole will allow to calculate the mass made in a chemical reaction. Take the chemical reaction below:

$$Mg + 2HCl \rightarrow MgCl_2 + H_2$$

This equation shows that one mole of magnesium reacts with two moles of hydrochloric acid to produce one mole of magnesium chloride and one mole of hydrogen gas. Suppose you started with 5 grams of magnesium, how much magnesium chloride would you make?

Step 1: Calculate the moles of the element or compound you were given in the equation:
5/24=0.21 moles of magnesium

Step 2: Look at the balanced equation, you must therefore have 0.21 moles of magnesium chloride, as the ration between magnesium and magnesium chloride is 1 to 1.

Step 3: Calculate the M_r of the relevant product: what you want to find is the M_r of magnesium chloride:
M_r of $MgCl_2$ =24+35.5+35.5= 94

Step 4: Now find the mass of that number of moles of the product
Mass = moles x M_r, so 0.21 x 94= 19.7 grams

Key Terms	Definitions
Mole	**6.02×10^{23} atoms of an element or molecules in a compound**
Avogadro's number	**6.02×10^{23}**
Relative Formula Mass	The total atomic mass of elements in compound

Equation	Meanings of terms in equation
$moles = \frac{mass}{M_r}$	*Mass is the mass of the substance in grams* *M_r is the relative formula mass of the compound (or use the relative atomic mass if it is an element)*

Calculating moles from masses -Higher Tier

If you know the mass of each reactant and product you can calculate a balanced equation from the masses, for example: Calculate the balanced equation when 12 grams of magnesium reacts completely with 19.25g of HCl, to make 99 grams of $MgCl_2$ and 1 gram of H_2

$$Mg + HCl \rightarrow MgCl_2 + H_2$$

Step 1: work out the moles of each reactant and product.
Mg=12/24= 0.5 HCl=19.25/38.5= 0.5 MgCl2 =99/99 =1 H2 ½ = 0.5
Step 2 divide through by the smallest number

Mg=0.5/0.5=1 HCl=0.5/0.5 = 1 $MgCl_2$ =1/0.5=2 H_2 ½ = 0.5/0.5=1

Step 3 write the balanced equation:

$$Mg + HCl \rightarrow 2MgCl_2 + H_2$$

Chemistry Knowledge Organiser
C4 - Chemical calculations

% Yield

In reactions in chemistry it is very rare that we make the exact mass predicted by calculation, for a variety of reasons we often make a lot less. The equation to calculate percentage yield is outlined in the equation box. **A percentage yield is always 100% or less**, the law of conservation of mass states that we cannot make mass in a chemical reaction.

It is extremely rare that the yield of a chemical reaction is 100% reasons for this are:

- The reaction is reversible and may not go to completion
- There may be side reactions
- Some maybe lost when the product is transferred from the reaction vessel

Atom Economy

Some reactions make more than one product, atom of these products will be waste products. The atom economy is a measure of the atoms that form useful products. Like percentage yields we express atom economy as a percentage so that comparisons can be easily made between reactions.

For example below two ways of making hydrogen are outlined:

1. $Zn + 2HCl \rightarrow ZnCl_2 + H_2$

M_r of $H_2 = 1 + 1 = 2$

M_r of $ZnCl_2 = 65 + 35.5 + 35.5 = 136$

Atom economy = $^{2}/_{136 + 2} \times 100 = {}^{2}/_{138} \times 100 = 1.45\%$ Very low atom economy

2. $CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$

M_r of $H_2 = 1 + 1 = 2$

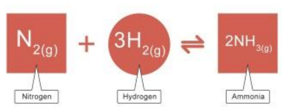
M_r of $CO_2 = 12 + 16 + 16 = 44$

Atom economy = $^{4 \times 2}/_{44 + (4 \times 2)} \times 100 = {}^{8}/_{52} \times 100 = 15.4\%$ Higher atom economy

In the second example the atom economy is higher, therefore in terms of atom economy reaction 2 is better. Chemists often need to balance atom economy and percentage yield. A poor atom economy is bad for a number of reasons:

1. A lot of reactant is wasted, this costs money.
2. The waste products have to be disposed of, this can be expensive. Some companies try to get around this problem by reusing the waste product.

The best reactions in terms of atom economy are those that only make one product, for example the Haber process, the atom economy here is 100%:



Key Terms	Definitions
Yield	The amount of product made in a chemical reaction
Atom Economy	The percentage of atoms that form useful products
Limiting Reagent	The reagent which is used up first in a chemical reaction.

Equation	Meanings of terms in equation
$\% \text{ yield} = \frac{Mass\ of\ products}{Mass\ of\ theoretical\ producti} \times 100$	*Mass of products is the mass made in a chemical reaction* *Mass of theoretical products is the mass we expected to make based on calculations* *Both these masses must be in the same unit.*
$\text{Atom economy} = \frac{Reltive\ formula\ mass\ of\ DESIRED\ roducts}{Total\ relative\ formula\ mass\ of\ products} \times 100$	*See the previous page for how to calculate relative formula mass*

Limiting Reagent

When a chemical reaction is carried out, one or more reagents are in excess and one reagent is the limiting reagent. The **limiting reagent** is the reagent which is used up first in a chemical reaction, if all of this reagent is used up the reaction can no longer continue, for example, if a tiny amount of sodium is dropped into a large bowl of water there are a lot more water particles that there are sodium atoms. We therefore say that the sodium is the **limiting reagent** and the water is in **excess.**

The amount of product formed is **directly proportional** to the amount of limiting reagent. Therefore if you double the amount of limiting reagent you will get double the amount of product.

Chemistry Knowledge Organiser
C4 - Chemical calculations – triple students only

Titration Calculations

We can use the information that we get from a titration to work out the concentration of an alkali or acid. For example a titration was carried using hydrochloric acid and sodium hydroxide, the equation for this reaction is:

$$HCl + NaOH \rightarrow NaCl + H_2O$$

This means that one mole of hydrochloric acid will neutralise 1 mole of sodium hydroxide.

Therefore we can calculate the following:

27.5 cm^3 of 0.2 mol/dm^3 hydrochloric acid is needed to titrate 25.0 cm^3 of sodium hydroxide solution. What is the concentration of the sodium hydroxide solution?

Step 1: Convert all volumes to dm^3

27.5 cm^3 = 27.5 ÷ 1000 = 0.0275 dm^3

25.0 cm^3 = 25.0 ÷ 1000 = 0.025 dm^3

Step 2: Calculate the number of moles of the substance where the volume and concentration are known

number of moles = concentration × volume

number of moles of hydrochloric acid = 0.2 × 0.0275 = 0.0055 mol (5.5×10^{-3} mol)

Step 3: Calculate the unknown concentration

We can say that 0.0055 mol of acid will react with 0.0055 mol of alkali

concentration of alkali = moles ÷ volume = 0.0055 ÷ 0.025 = **0.22 mol/dm^3**

Moles of a Gas

We know that one mole of any gas occupies 2**4 dm^3 at room temperature and pressure.** Room Temperature and pressure is defined as 20 ˚c and 1 atm of pressure. Therefore if we know the volume that the gas occupies, we can divide this number by 24 and this will give us the number of moles. For example if we had 12 dm^3 of argon gas at room temperature and pressure, then to find out the moles we would simply do 12/24= 0.5 moles.

We can also use balanced equations to work out volumes of gas, for example:

$2CO + O_2 \rightarrow 2CO_2$

If we start with 24 dm^3 of oxygen we will make 48 dm^3 of carbon dioxide, as the ration in the equation shows that one mole of oxygen will make 2 moles of carbon dioxide.

You may also be asked to calculate the volume a gas occupies after being given the mass in the equation. For Example: What volume would 2 grams of carbon dioxide occupy at room temperature and pressure?

Step 1: Calculate the moles of carbon dioxide= 2/44= 0.05 moles

Step 2: Multiply this number by 24 as we know 1 mole occupies 24 dm^3 0.05x24= 1.2 dm^3

Key Terms	Definitions
Decimetre	A unit of volume, often used in chemistry. It is the same as 1000 cm^3
Atmosphere	A unit of gas pressure. It is the same as 101325 Pa

Equation	Meanings of terms in equation
$\text{Volume} = \frac{\text{Mass of gas}}{\text{Mr of gas}} \times 24$	*Mass of gas in grams* *Volume of gas will be in* dm^3

Limiting Reagent

When a chemical reaction is carried out, one or more reagents are in excess and one reagent is the limiting reagent. The **limiting reagent** is the reagent which is used up first in a chemical reaction, if all of this reagent is used up the reaction can no longer continue, for example, if a tiny amount of sodium is dropped into a large bowl of water there are a lot more water particles that there are sodium atoms. We therefore say that the sodium is the **limiting reagent** and the water is in **excess.**

The amount of product formed is **directly proportional** to the amount of limiting reagent. Therefore if you double the amount of limiting reagent you will get double the amount of product.

Chemistry Knowledge Organiser
C4 - Chemical calculations

Key Terms	Definitions
Concentration	A measure of the number of moles or mass in a given volume.
Titration	An experimental techniques where unknown concentrations of solutions can be found.
Burette	A piece of apparatus used to accurately measure volumes of solution.

Concentration

Most chemical reactions are done in solution. The concentration can be measured in grams per dm^3

For example what is the concentration in grams/dm^3 of 2.4 grams of sodium chloride dissolved in 0.5 dm^3 of water?

Conc= Mass/Vol

Conc= 2.4/0.5

Conc= 4.8 g/dm^3

In Chemistry we use dm^3 (decimetres cubed) to measure volume, a decimetre cubed is the same as a litre or 1000 cm^3.

However it is far more common to calculate a concentration in moles per dm^3. This is sometimes written as M.
For example, what is the concentration of 2.4 grams of sodium chloride dissolved in 0.5 dm^3 in mol/dm^3?
Moles of NaCl= 2.4/58.5= 0.041 moles

Conc=moles/vol – triple students only

Conc= 0.041/0.5

Conc=0.082 mol/dm^3

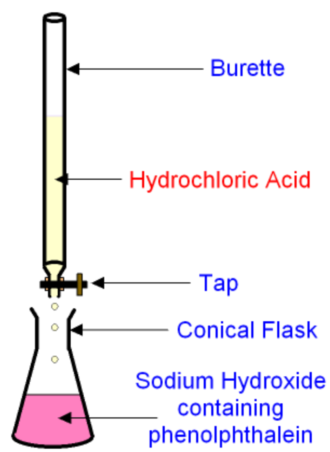
It is also possible to convert between mol/ dm^3 and g/ dm^3 for example. If I had 0.5 mol/ dm^3 HCl solution. We can work out the concertation in g/ dm^3:
Step 1: Work out the Mr of HCl: 35.5+1= 36.5
Step 2= Mass= Moles x Mr= 36.5 x 0.5 = 18.25 g/ dm^3

Equation	Meanings of terms in equation
$\text{conc} = \frac{mass}{vol}$	*Mass is the mass of the solute in grams* *Vol is the volume of the solventin* dm^3 *Conc is the concentration in* grams/dm^3
$\text{conc} = \frac{Moles}{volume}$	*Triple students only –* *Moles is the number of moles of the solute* *Vol is the volume of the solution in* dm^3 *Conc is the concentration in* grams/dm^3

Titrations – triple students only

Titrations are used to find out an **unknown concentration of a solution**, this is often used to find out the concentration of an acid or an alkali in a neutralisation reaction. To carry out a titration to find the concentration of an alkali you need to do the following:

1. A pipette is used to measure 25 cm^3 of alkali, this is then transferred to a conical flask.
2. 3-4 Drops of indicator is added (phenolphthalein).
3. An acid of known concentration is placed in the burette
4. The solution from the burette is allowed to slowly run into the conical flask. As the end point approaches the acid is added one drop at a time. When phenolphthalein is used as an indicator, the end point is where the solution turns from colorless to pink.
5. The volume of acid used from the burette is noted to calculate the concentration of the alkali in the conical flask. See the next page for how to carry out these calculations.



Indicators – triple students only

For titrations universal indicator is not a suitable indicator to use. As the colour changes are too gradual. For a titration, a sharp colour change is required . Suitable indicators are listed below.

	In acid	In alkali
Litmus	Red	Blue
Methyl Orange	Red	Yellow
Phenolphthalein	Colourless	Pink