1. Formulae, equations and amounts 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

For most calculations we will do at AS we will use the following 3 equations

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

1. For pure solids and gases

$$\text{amount} = \frac{\text{mass}}{\text{MolarMass}}$$

Unit of Mass: grams
Unit of amount : mol

2. For Gases

Gas Volume (dm^3)= amount x 24

This equation give the volume of a gas at room pressure (1atm) and room temperature 25^oC.

3. For solutions

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

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

Converting volumes

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

It is usually best to give your answers to 3sf

Typical mole calculations

Some Simple calculations using above equations

Example 1: What is the amount, in mol, in 35g of $CuSO_4$?

amount = mass/Mr

= 35/ (63.5 + 32 +16 x4)

= 0.219 mol

Example 2: What is the concentration of solution made by dissolving 5g of Na_2CO_3 in 250 cm^3 water?

amount = mass/Mr

= 5 / (23.1 x2 + 12 +16 x3)

= 0.0472 mol

conc= amount/Volume

= 0.0472 / **0.25**

= 0.189 mol dm^{-3}

Example 3 : What is the volume in dm^3 at room temperature and pressure of 50g of Carbon dioxide gas ?

amount = mass/Mr

= 50/ (12 + 16 x2)

= 1.136 mol

Gas Volume (dm^3)= amount x 24

= 1.136 x 24

= 27.26 dm^3 (or 27.3 dm^3 to 3 sig fig)

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

amount = mass/Ar

= 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 5 : How many chloride ions are there in a 25.0 cm^3 of a solution of magnesium chloride of concentration 0.400 $moldm^{-3}$?

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}

Parts per million (ppm)

Concentrations can be given also in parts per million. This is often used for gases in the atmosphere or in exhausts, and pollutants in water.

$$\text{parts per million (ppm) of substance, by mass} = \frac{\text{mass of substance in mixture}}{\text{total mass of mixture}} \times 1000\,000$$

Example 6 : Blood plasma typically contains 20 parts per million (ppm) of magnesium, by mass. Calculate the mass of magnesium, in grams, present in 100 g of plasma.

$$\text{parts per million (ppm) of substance, by mass} = \frac{\text{mass of substance in mixture}}{\text{total mass of mixture}} \times 1000\,000$$

$$20 = \frac{\text{mass of substance in mixture}}{100} \times 1000\,000$$

mass of substance in mixture = 20 x100/1000 000
= 2×10^{-3} g

Empirical Formula

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

General method

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

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

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

These whole numbers will be the empirical formula.

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

1. masses of each element in the compound

2. percentage mass of each element in the compound

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

Step1: Divide each mass by the atomic mass of the element

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 (Mr) work out how many times the mass of the empirical formula fits into the Mr.

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

C_3H_6O has a mass of 58

The empirical formula fits twice into M_r of 116

So molecular formula is $C_6H_{12}O_2$

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

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 9: What mass of Carbon dioxide would be produced from heating 5.5 g of sodium hydrogencarbonate?
$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$
Step 1: work out amount, in mol, of sodium hydrogencarbonate
amount = mass / Mr
= 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: work out mass of CO_2
Mass = amount x Mr
= 0.0328 x 44.0
=1.44g

Example 10: What mass of Copper would react completely with 150 cm^3 of 1.6M nitric acid?
$3Cu + 8HNO_3 \rightarrow 3Cu(NO_3)_2 + 2NO + 4H_2O$

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

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

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

Example 11: What volume in cm^3 of oxygen gas would be produced from the decomposition of 0.532 g of potassium chlorate(V)?
$2KClO_3 \rightarrow 2 KCl + 3O_2$
Step 1: work out amount, in mol, of potassium chlorate(V)?
amount = mass / Mr
= 0.532 /122.6
= 0.00434 mol

Step 2: use balanced equation to give amount in mol of O_2
2 moles $KClO_3$: 3 moles O_2
So 0.00434 HNO_3 : 0.00651moles O_2
Step 3: work out volume of O_2

Gas Volume (dm^3)= amount x 24

= 0.00651 x 24

= 0.156 dm^3

= 156 cm^3

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)

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

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

Example 12 If one burnt 500 cm^3 of methane at 1atm and 300K what volume of Oxygen would be needed and what volume of CO_2 would be 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
$500 cm^3$	$1 dm^3$	$500 cm^3$

Simply multiply gas volume x2

Example 13
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 ?

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

total volume of gases produced = $750 cm^3$

% Yield

percentage yield = $\dfrac{\textbf{actual yield}}{\textbf{theoretical yield}}$ **x 100**

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

Example 14: 25g of Fe_2O_3 was reacted and it produced 10g of Fe. What is the percentage yield?

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

First calculate maximum mass of Fe that could be produced

Step 1: work out amount in mol of Iron oxide
amount = mass / Mr
=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 Mr
= 0.313 x 55.8
=17.48g

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

% Atom Economy

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

Do take into account balancing numbers when working out % atom economy.

Example 15: What is the % atom economy for the following reaction where Fe is the desired product assuming the reaction goes to completion?

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

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

$= 45.8\%$

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

Making Salts

A **Salt** is formed when the H^+ ion of an acid is replaced by a metal ion or an ammonium ion

The most common strong acids are :
Hydrochloric (HCl), sulphuric (H_2SO_4) and nitric (HNO_3) acid;

Neutralisation reactions form salts

Bases neutralise acids. Common bases are metal oxides, metal hydroxides and ammonia.

An Alkali is a soluble base that releases OH^- ions in aqueous solution;
The most common alkalis are sodium hydroxide (NaOH), potassium hydroxide (KOH) and aqueous ammonia (NH_3)

Common Neutralisation Reaction Equations

ACID + BASE → SALT + WATER

$HCl + NaOH \rightarrow NaCl + H_2O$

$2HNO_3 + Mg(OH)_2 \rightarrow Mg(NO_3)_2 + 2H_2O$

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

$2HCl + CaO \rightarrow CaCl_2 + H_2O$

$HCl + NH_3 \rightarrow NH_4Cl$

acid + metal → salt + hydrogen
$2HCl + Mg \rightarrow MgCl_2 + H_2$

Acid + Carbonate → Salt + Water + Carbon Dioxide

$H_2SO_4 + K_2CO_3 \rightarrow K_2SO_4 + CO_2 + H_2O$

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

$2HCl + CaCO_3 \rightarrow CaCl_2 + CO_2 + H_2O$

Observations : In carbonate reactions there will be Effervescence due to the CO_2 gas evolved and the solid carbonate will dissolve. The temperature will also increase.

Method for preparing a soluble salt

If using an insoluble base, metal or solid carbonate

- Add solid base to acid (gently heat to speed up reaction
- Filter off excess solid base
- Heat filtrate solution until volume reduced by half
- Leave solution to cool and allow remaining water to evaporate
- Slowly and crystals to form
- Filter or pick out crystals
- Leave to dry and put crystals between filter

Use excess solid base/ metal/carbonate to ensure all **acid** reacts/neutralises and that the product is neutral

The percentage yield of crystals will be less than 100% because some salt stays in solution. There will also be losses on transferring from one container to another and a loss on filtering.

If using an soluble base

An indicator can be used to show when the acid and alkali have completely reacted to produce a salt solution using the titration method. Then repeat reaction without indicator using the same volumes. Then follow above method from the reducing volume of solution stage to evaporate neutralised solution to get crystals of salt

Insoluble salts

Insoluble salts can be made by mixing appropriate solutions of ions so that a **precipitate** is formed
Lead nitrate (aq) + sodium chloride (aq) → **lead chloride (s)** + sodium nitrate (aq)
These are called **precipitation** reactions. A **precipitate is a solid**

When making an insoluble salt, normally the salt would be removed by **filtration,** washed with distilled water to remove soluble impurities and then **dried on filter paper**

Writing Ionic equations for precipitation reactions

We usually write ionic equations to show precipitation reactions. Ionic equations only show the ions that are reacting and leave out spectator ions.

Spectator ions are ions that are not
- Not changing state
- Not changing oxidation number

Take full equation

$$Pb(NO_3)_2\ (aq) + 2NaCl\ (aq) \rightarrow PbCl_2\ (s) + 2\ NaNO_3\ (aq)$$

Separate (aq) solutions into ions

$$Pb^{2+}_{(aq)} + 2NO_3^-{}_{(aq)} + 2Na^+{}_{(aq)} + 2Cl^-{}_{(aq)} \rightarrow PbCl_{2\ (s)} + 2\ Na^+{}_{(aq)} + 2NO_3^-{}_{(aq)}$$

Cancel out spectator ions leaving ionic equation

$$Pb^{2+}_{(aq)} + 2Cl^-{}_{(aq)} \rightarrow PbCl_{2\ (s)}$$

Ionic equations for reactions of acids with metals, carbonates, bases and alkalis

Ionic Equations

acid + metal → salt + hydrogen
$2HCl_{(aq)} + Mg(s) \rightarrow MgCl_2(aq) + H_2(g)$ ⟶ $2H^+_{(aq)} + Mg_{(s)} \rightarrow Mg^{2+}_{(aq)} + H_{2(g)}$

acid + alkali (NaOH) → salt + water
$2HNO_2(aq) + Ba(OH)_2(aq) \rightarrow Ba(NO_2)_2(aq) + 2H_2O_{(l)}$ ⟶ $H^+_{(aq)} + OH^-_{(aq)} \rightarrow H_2O_{(l)}$

acid + carbonate (Na_2CO_3) → salt + water + CO_2
$2HCl(aq) + Na_2CO_3(aq) \rightarrow 2NaCl(aq) + H_2O(l) + CO_{2(g)}$ ⟶ $2H^+_{(aq)} + CO_3^{2-}{}_{(aq)} \rightarrow H_2O_{(l)} + CO_{2(g)}$

Example
The equation representing the reaction between copper(II) oxide and dilute sulfuric acid is
$CuO(s) + H_2SO_4(aq) \rightarrow CuSO_4(aq) + H_2O(l)$
What is the ionic equation?
Only sulphate ion is a spectator ion in this case because it's the only ion not changing state
$CuO(s) + 2H^+ \rightarrow Cu^{2+}(aq) + H_2O(l)$

Hazards and Risks

A **hazard** is a substance or procedure that can has the potential to do harm.
Typical hazards are toxic/flammable /harmful/ irritant /corrosive /oxidizing/ carcinogenic

RISK: This is the probability or chance that harm will result from the use of a hazardous substance or a procedure

In the laboratory we try to minimise the risk

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.

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

Using a gas syringe

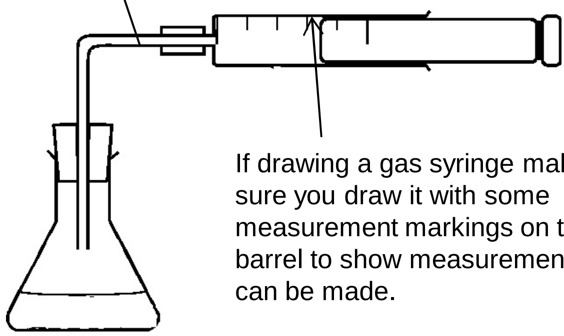
Gas syringes can be used for a variety of experiments where the volume of a gas is measured, possibly to work out moles of gas or to follow reaction rates.

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 molar gas volume

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.

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.

Making a solution

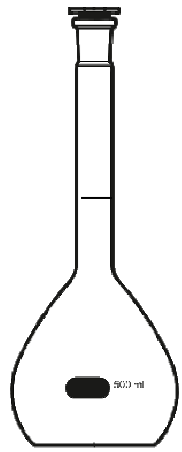
•Weigh required mass of solute in a weighing bottle.

• Tip contents into a beaker and add100cm^3 of distilled water. 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.

Weighing can be made more accurate by weighing bottle again after it has been emptied into the beaker- or alternatively the weighing bottle could be 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.

Errors

Calculating apparatus errors
Each type of apparatus has a sensitivity error

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

Calculate the percentage error for each piece of equipment used by

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

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

To calculate the maximum percentage apparatus error in the final result add all the individual equipment errors together.

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

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

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

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

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

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

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

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 16
$Na_2SO_4 . xH_2O$ 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

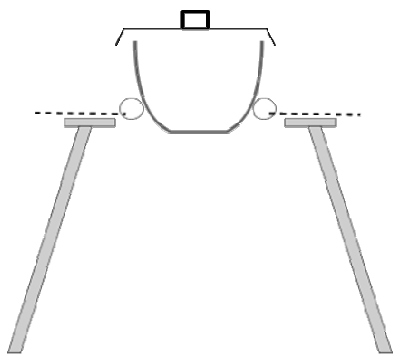
This method could be used for measuring mass loss in various thermal decomposition reactions and also for mass gain when reacting magnesium in oxygen.

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

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

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

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



Large amounts of hydrated calcium sulphate, such as 50g, should not be used in this experiment as the decomposition is 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 17. 3.51 g of hydrated zinc sulphate were heated and 1.97 g of anhydrous zinc sulphate were obtained.
Use these data to calculate the value of the integer *x* in $ZnSO_4.xH_2O$

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

Calculate moles of $ZnSO_4$ $= \frac{1.97}{161.5}$ = 0.0122

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

Calculate ratio of mole of $ZnSO_4$ to H_2O $= \frac{0.0122}{0.0122}$ =1 $= \frac{0.085}{0.0122}$ =7

X = 7