## 1.1 FORMULAE, EQUATIONS AND AMOUNT OF SUBSTANCE

### **Syllabus Specification:**

- a. know the terms 'atom', 'element', 'ion', 'molecule', 'compound', 'empirical formula' and 'molecular formula'
- b. know that the mole (mol) is the unit for the amount of a substance and be able to perform calculations using the Avogadro constant L  $(6.02 \times 1023 \text{ mol-1})$
- c. write balanced full and ionic equations, including state symbols, for chemical reactions
- d. understand the terms:
  - i 'relative atomic mass' based on the 12C scale
  - ii 'relative molecular mass' and 'relative formula mass', including calculating these values from relative atomic masses

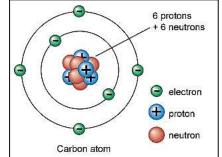
The term 'relative formula mass' should be used for compounds with giant structures.

- iii 'molar mass' as the mass per mole of a substance in q mol-1
- iv parts per million (ppm), including gases in the atmosphere
- e. calculate the concentration of a solution in mol dm-3 and g dm-3 Titration calculations are not required at this stage.
- f. be able to use experimental data to calculate empirical and molecular formulae
- g. be able to use chemical equations to calculate reacting masses and vice versa, using the concepts of amount of substance and molar mass
- h. be able to use chemical equations to calculate volumes of gases and vice versa, using:
  - i the concepts of amount of substance
  - ii the molar volume of gases
  - iii the expression pV = nRT for gases and volatile liquids
- i. be able to calculate percentage yields and percentage atom economies (by mass) in
- j. laboratory and industrial processes, using chemical equations and experimental results  $Atom\ economy = \frac{\frac{molar\ mass\ of\ the\ desired\ product}{sum\ of\ the\ molar\ masses\ of\ all\ products}}{\frac{sum\ of\ the\ molar\ masses\ of\ all\ products}{sum\ of\ the\ molar\ masses\ of\ all\ products}} \times 100\%$
- k. be able to determine a formula or confirm an equation by experiment, including evaluation of the data
- I. CORE PRACTICAL 1
  - Measurement of the molar volume of a gas.
- m. be able to relate ionic and full equations, with state symbols, to observations from simple test-tube experiments, to include:
  - i displacement reactions
  - ii typical reactions of acids
  - iii precipitation reactions
- n. Further suggested practicals:
  - i preparation of a salt and calculating the percentage yield of product, including the preparation of a double salt, such as ammonium iron(II) sulfate from iron, ammonia and sulfuric acid
  - ii determine a chemical formula by experiment, such as the formula of copper(II)oxide by reduction
  - iii determine a chemical equation by experiment, such as the reaction between lithium and water, or the reaction between magnesium and an acid
  - iv carry out and interpret the results of simple test-tube reactions, as outlined
  - in 1.12

### **MOTA**

An atom is the smallest, electrically neutral particle of an element that can take part in a chemical change. All atoms are made up of three sub-atomic particles; **protons**, **neutrons and electrons**.

- **Protons and neutrons** are together known as **nucleons** and are found in the **nucleus**.
- **Electrons** orbit around the nucleus in definite energy levels called **shells**.



#### **ELEMENT**

**Element**s are basically the simplest substances so they cannot be broken down using chemical reactions.

Example: neon

### **MOLECULE**

• Particle made of two or more atoms of the same element or different elements bonded together.

**Example**: Hydrogen (H<sub>2</sub>) – made of two hydrogen atoms.

Water (H<sub>2</sub>O) – made of two atoms of hydrogen and one atom of oxygen

### **COMPOUND**

Substance containing atoms of different elements combined together.

Example: H<sub>2</sub>O

**MONOATOMIC** – **elements** made up of single atoms.

Example: Helium (He)

**DIATOMIC** – **elements** and **comounds** made up of two atoms joined together

Example: nitrogen (N<sub>2</sub>)

**POLYATOMIC**: **elements** and **compounds** made up of several atoms joined

together.

*Example*: Phosporous (P<sub>4</sub>)

### ION

A species containing of one or more atoms joined together and having a positive or a negative charge.

**Cation:** ion with positive charge.

• Have fewer electrons than protons as electrons are removed from a neutral atom.

**Example:** Na<sup>+</sup> ion has 11 protons and 10 electrons.

**Anion:** ion with negative charge

Have more electrons than protons as electrons are added to a neutral atom.

**Example:** Cl<sup>-</sup> ion has 17 protons and 18 electrons.

Term	Diagram	Name	Symbol	Note
Element	Cu Cu	Copper	Cu	This is an element. All the atoms are same
Atom	He	Helium	Не	This is an atom of an element
Molecule	Br Br	Bromine	Br <sub>2</sub>	This is a molecule of an element. The atoms are the same
Compound	H Br	Hydrogen bromide	HBr	This is a molecule of a compound. The atoms are different.
Ion	_O_C_O_	Carbonate	CO <sub>3</sub> <sup>2-</sup>	This is an ion. There are two negative charges shown.

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1.	1. Classify each of these symbols and formulae as atoms, molecules or ions		
	Ne	<i>CO</i> <sub>2</sub>	
	H+	$S_6$	
	Al <sup>3+</sup>	$N_2$	
2.	Which of these formulae represent	t elements, compounds or neither elements no	
	compounds? Explain your answer.		
	<i>Br</i> <sub>2</sub> :		
	$H_2O_2$ :		
	NO <sub>3</sub> :		
	03:		
	CaO:		

# WRITING CHEMICAL EQUATIONS

#### **FORMULA**

A formula represents one molecule of a compound, or the simplest ratio of the ions present. As with symbols, a formula represents a single particle or one mole particles.

• Valency is a numerical measure of the combining power of an atom/ion. Below is a list of common valencies that will help in constructing formulae.

1	hydrogen	H⁺	chloride	Cl-
	sodium	Na⁺	bromide	Br⁻
	potassium	K⁺	iodide	I-
	lithium	Li⁺	hydroxide	OH-
	rubidium	Rb⁺	nitrate	NO <sub>3</sub> -
	caesium	Cs⁺	nitrite	NO <sub>2</sub> -
	copper(I)	Cu⁺	hydrogen carbonate	HCO₃⁻
	silver(I)	Ag⁺	hydrogen sulfate	HSO <sub>4</sub> -
	ammonium	$NH_4^{\scriptscriptstyle \dagger}$		
2	calcium	<i>C</i> a <sup>2+</sup>	sulfate	SO <sub>4</sub> <sup>2-</sup>
	barium	Ba <sup>2+</sup>	sulfite	SO <sub>3</sub> <sup>2-</sup>
	magnesium	Mg <sup>2+</sup>	sulfide	S <sup>2-</sup>
	zinc	$Zn^{2+}$	oxide	O <sup>2-</sup>
	iron(II)	Fe <sup>2+</sup>	carbonate	CO3 <sup>2-</sup>
	cobalt	<i>C</i> o <sup>2+</sup>		
	manganese(II)	$Mn^{2+}$		
	copper(II)	Cu <sup>2+</sup>		
3	aluminium	Al <sup>3+</sup>	phosphate	PO <sub>4</sub> <sup>3-</sup>
	iron(III)	Fe <sup>3+</sup>		

#### **WORKED EXAMPLE 1:**

What is the formula of Magnesium Chloride?

MgCl<sub>2</sub>

If the numeral charges are the same on the ions they can be cancelled out so the ratio is one cation and one anion

#### WORKED EXAMPLE 2:

What is the formula of Calcium hydrogen carbonate?

 $Ca(HCO_3)_2$ 

If the numeral charges are not the same the numbers of each ion have to be worked out so that the total positive charge equals total negative charge.

### WRITING AN EQUATION FROM A DESCRIPTION

- 1. Write the formulae of the reactants and products.
- 2. Balance the equation. You need to add up the numbers of all atoms to make sure that, for each element, the totals are the same on both the left and the right side of the equation.

### **Example:**

$$CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O$$

There is one carbon, one calcium, two hydrogen and four oxygen atoms on each side, so the equation is already balanced.

Most equations are balanced using whole number coefficients, but using fractions or decimals usually acceptable.

$$C_4H_{10} + 6\frac{1}{2}O_2 \rightarrow 4CO_2 + 5H_2O$$

#### **USING STATE SYMBOLS**

Many chemical equations include state symbols.

- (s) = solid
- (l) = liquid
- (g) = gas
- (aq) = aqueous (dissolved in water)

## **IONIC EQUATIONS**

Ionic equations show any atoms and molecules involves, but only the ions that react together, and not the **spectator ions** (an ion that is there both before and after the reaction but is not involved in the reaction)

- 1. Start with the full equation for the reaction
- 2. Replace the formulae of ionic compounds by their separate ions
- 3. Delete any ions that appear identically on both sides.

## Worked example:

What is the simplest ionic equation for the neutralization of sodium hydroxide solution by dilute nitric acid?

The full equation is

$$NaOH(aq) + HNO_3(aq) \rightarrow NaNO_3(aq) + H_2O(l)$$

You should now consider which of these species are ionic and replace them with ions. In this example, the first three compounds are ionic:

$$Na^{+}(aq) + OH^{-}(aq) + H^{+}(aq) + NO_{3}^{-}(aq) \rightarrow Na^{+}(aq) + NO_{3}^{-}(aq) + H_{2}O(l)$$

After deleting the identical ions, the equation becomes:

$$H^+$$
 (aq) +  $OH^-$ (aq)  $\to H_2O(1)$ 

### **SOLUBILITY OF IONIC COMPOUNDS**

Many ionic solids are soluble in water:

- ✓ All group 1 metal compounds are soluble
- ✓ All ammonium compounds are soluble
- ✓ All nitrates are soluble.
- ✓ All chlorides are soluble, apart from silver chloride and lead (II) chloride
- ✓ All sulfates are soluble, apart from strontium sulphate, barium sulphate and lead(II) sulphate. (calcium sulphate is only very slightly soluble)

Some types of ionic solids are mostly insoluble in water:

- All carbonates are insoluble, apart from group 1 and ammonium carbonates
- \* All hydroxides are insoluble, apart from group 1 hydroxides, ammonium hydroxide and barium hydroxide (calcium and strontium hydroxides are slightly soluble).

#### **CHECKPOINT 2**

- 1. What is the simplest ionic equation for the reaction that occurs when solutions of lead(ii)nitrate and sodium sulfate react together to perform a precipitate of lead(ii)sulfate and a solution of sodium nitrate.
  - 2. Carbondioxide reacts with calcium hydroxide solution to form water and a precipitate of calcium carbonate. Write the simplest ionic equation.

#### **CHECKPOINT 3**

1. Sodium thiosulfate ( $Na_2S_2O_3$ ) solution reacts with dilute hydrochloric acid to form a precipitate of sulphur, gaseous sulphur dioxide and a solution of sodium chloride. Write an equation, including state symbols, for this reaction.

2. Solutions of ammonium sulfate and sodium hydroxide are warmed together to form sodium sulfate solution, water and ammonia gas. Write the simplest ionic equation for this reaction.

## TYPICAL REACTIONS OF ACIDS

### Acids with metals

- **General equation**: metal + acid → salt + hydrogen
- *Observation*: bubbles of hydrogen form
- Reactive metals react this way. Magnesium and copper does not.

### Example:

$$Mg + 2HCl \rightarrow MgCl_2 + H_2$$
  
 $Mg(s) + 2H^+(aq) \rightarrow Mg^{2+}(aq) + H_2(g)$ 

## Acids with metal oxides & insoluble metal hydroxides

- $metal\ oxide + acid \rightarrow salt + water$ • General equation :  $metal\ hydroxide + acid \rightarrow salt + water$
- *Observation*: formation of a solution
- Reactivity of the metal does not matter because in the reactant is present as metal ions, not metal atoms.

### Example:

CuO + H<sub>2</sub>SO<sub>4</sub> 
$$\rightarrow$$
 CuSO<sub>4</sub>+ H<sub>2</sub>O  
CuO(s) + 2H<sup>+</sup>(aq)  $\rightarrow$  Cu<sup>2+</sup>(aq) + H<sub>2</sub>O(l)  
Zn(OH)<sub>2</sub> + H<sub>2</sub>SO<sub>4</sub>  $\rightarrow$  ZnSO<sub>4</sub> + 2H<sub>2</sub>O  
Zn(OH)<sub>2</sub> (s) + 2H<sup>+</sup>(aq)  $\rightarrow$  Zn<sup>2+</sup>(aq) + 2H<sub>2</sub>O(l)

These reaction can be classified as neutralisation reactions because the H<sup>+</sup> ions react with O<sup>2-</sup> or OH<sup>-</sup> ions.

#### Acids with alkalis

- Alkali metal hydroxide dissolved in water
- **General equation**:  $alkali + acid \rightarrow salt + water$
- *Observation:* temperature rise.

### Example: Sodium hydroxide reacting with phosphoric acid

NaOH + 
$$H_3PO_4 \rightarrow NaH_2PO_4 + H_2O$$
  
2NaOH +  $H_3PO_4 \rightarrow Na_2HPO_4 + 2H_2O$   
3NaOH +  $H_3PO_4 \rightarrow Na_3PO_4 + 3H_2O$ 

$$Zn(OH)_2 + H_2SO_4 \rightarrow ZnSO_4 + 2H_2O$$
  
 $Zn(OH)_2 (s) + 2H^+(aq) \rightarrow Zn^{2+}(aq) + 2H_2O(l)$ 

There are three replaceable hydrogens in phosphoric acid. The salt formed depends on the relative amounts of acid and alkali used.

The ionic equation for all these reactions is:

$$H^+(aq) + OH^-(aq) \rightarrow H_2O(l)$$

 These reaction can be classified as neutralisation reactions because the H<sup>+</sup> ions react with OH<sup>-</sup>ions.

## **Acids with carbonates**

- **General equation**:  $metal\ carbonate + acid \rightarrow salt + water + carbondioxide$
- *Observation:* bubbles of carbondioxide gas form.

If the salt formed is soluble, then a solution forms.

Example: lithium carbonate reacting with hydrochloric acid

$$\text{Li}_2\text{CO}_3 + 2\text{HCl} \rightarrow 2\text{LiCl} + \text{H}_2\text{O} + \text{CO}_2$$
  
 $\text{CO}_3^{2-}$  (aq) + 2H<sup>+</sup>(aq)  $\rightarrow$  H<sub>2</sub>O(l) + CO<sub>2</sub> (g)

These reaction can be classified as neutralisation reactions because the H<sup>+</sup> ions react with  $CO_3^{2-}$  ions.

## Acids with hydrogencarbonates

- *General equation*:  $metal hydrogen carbonate + acid \rightarrow salt + water + carbondioxide$
- **Observation:** bubbles of carbondioxide gas form.

If the salt formed is soluble, then a solution forms.

Example: lithium carbonate reacting with hydrochloric acid

LiHCO<sub>3</sub> + HCl 
$$\rightarrow$$
 LiCl + H<sub>2</sub>O + CO<sub>2</sub>  
HCO<sub>3</sub><sup>-</sup> (aq) + H<sup>+</sup>(aq)  $\rightarrow$  H<sub>2</sub>O(l) + CO<sub>2</sub> (g)

These reaction can be classified as neutralisation reactions because the H<sup>+</sup> ions react with HCO<sub>3</sub> ions.

## **Test for carbonates and hydrogen carbonates**

**Test:** add an aqueous acid

*Observation:* bubbles of a gas which turns limewater milky is produced.

The gas is carbondioxide.

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GNE	UNP		11 7

- 1. Write full equations for the reactions between
  - a) zinc and sulfuric acid

b) aluminium oxide and hydrochloric acid

- 2. Write the simplest ionic equations for the reactions between
  - a) zinc and hydrochloric acid

b) magnesium carbonate and nitric acid

# **DISPLACEMENT REACTIONS**

• Displacement reaction is a reaction in which one element replaces another, less reactive, element in a compound.

# **Displacement reactions involving metals**

There are types of metal displacement.

1. Metal displacement in aqueous solution

Example:

$$Mg(s) + CuSO_4(aq) \rightarrow Cu(s) + MgSO_4(aq)$$

2. Metal displacement in solid state

Example:

$$Al(s) + Fe_2O_3(s) \rightarrow 2Fe(s) + Al_2O_3(s)$$

## 1. Metal displacement in aqueous solution

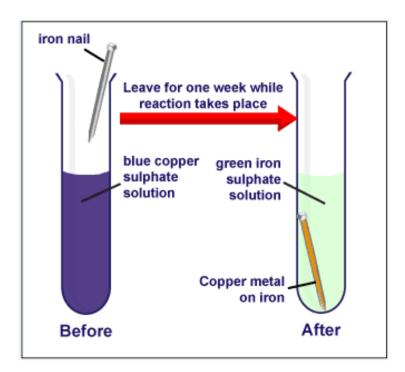
**Example 1:**  $Mg(s) + CuSO_4(aq) \rightarrow Cu(s) + MgSO_4(aq)$ 

- When magnesium metal is added to copper(ii) sulfate solution, the blue colur becomes paler.
- If an excess of magnesium is added, the solution becomes colourless, as magnesium sulfate forms.
- Magnesium changes its appearance from silvery to brown as copper forms.

**Ionic equation**:  $Mg(s) + Cu^{2+}(aq) \rightarrow Cu(s) + Mg^{2+}(aq)$ 

- This is a redox reaction.
- Electrons are transferred from magnesium atoms to copper(ii)ions, so magnesium atoms are oxidised (loss of electrons)and copper(ii)ions are reduced(gain of electrons)

## Example: 2



## 2. Metal displacement in solid state

**Example 1:**  $Al(s) + Fe_2O_3(s) \rightarrow 2Fe(s) + Al_2O_3(s)$ 

- This reaction is used in railway industry to join rails together using the thermite method.
- A mixture of aluminium and iron(iii) oxide is positioned just above the place where the two rails are to be joined.
- A magnesium fuse is lit, and the reaction given above occurs.
- It is so exothermic that the iron is formed as a molten metal, which flows into the gap between the two rails.
- The molten iron cools, joining the rails together.

**Ionic equation**:  $2Al(l) + 2Fe^{3+}(l) \rightarrow 2Fe(l) + 2Al^{3+}(l)$ 

- This is a redox reaction.
- Electrons are transferred from aluminium atoms to iron(iii)ions, so aluminium atoms are oxidised (loss of electrons) and iron(iii)ions are reduced(gain of electrons)



# Displacement reactions involving Halogens

More reactive halogens can displace less reactive halogens from their compounds.

*Example:* chlorine will displace bromine from a potassium bromide solution.

$$Cl_2(aq) + 2KBr(aq) \rightarrow Br_2(aq) + 2KCl(aq)$$
  
 $Cl_2(aq) + 2Br(aq) \rightarrow Br_2(aq) + 2Cl(aq)$ 

• As with the metal displacement reaction, this is a redox reaction. Electrons are transferred from bromide ions to chlorine, so bromide ions are oxidised and chlorine is reduced.

#### **CHECKPOINT 5**

1. Iron metal reacts with silver nitrate in a displacement reaction to form silver and iron(ii)nitrate. Write a full equation, an ionic equation and a simplified ionic equation for this reaction. Include state symbols in all your equations.

2. A mixture of zinc metal and copper(ii)oxide is ignited, causing an exothermic reaction to occur. Write a full equation, an ionic equation and a simplified ionic equation for this reaction. Do not include state symbols in your answer.

## **PRECIPITATION REACTIONS**

Precipitation reaction is a reaction in which an insoluble solid is formed when two solutions are mixed.

# **Chemical tests**

### Carbondioxide

• This is a precipitation reaction.

**Test:**  $CO_2$  is bubbled through calcium hydroxide solution  $(Ca(OH)_2)$  (Lime water).

**Observation:** white precipitate (calcium carbonate) forms.

**Equation:** 

 $Ca(OH)_2(aq) + CO_2(g) \rightarrow CaCO_3(s) + H_2O(l)$ 

### **Sulfates**

• This is a precipitation reaction.

**Test:** add barium ions(usually barium chloride or barium nitrate) to sulfate solution.

**Observation:** white precipitate (barium sulfate) forms.

**Equation:** 

$$Na_2SO_4(aq) + BaCl_2(aq) \rightarrow BaSO_4 + 2NaCl(aq)$$

$$SO_4^{2-}(aq) + Ba^{2+}(aq) \rightarrow BaSO_4(s)$$

## **Halides**

• This is a precipitation reaction.

**Test:** add silver ions to solution with halide ions

**Observation:** precipitate forms (silver halide)

**Equation:** 

$$NaCl(aq) + AgNO_3(aq) \rightarrow AgCl(s) + NaNO_3(aq)$$

$$Cl^{-}(aq) + Ag^{+}(aq) \rightarrow AgCl(s)$$

## Relative atomic mass (Ar)

• Relative atomic mass (A<sub>r</sub>) of an element is the weighted mean (average) mass of an atom compared to  $\frac{1}{12}$ th of the mass of an atom of  $^{12}$ C

Mean mass of an atom of an element 
$$A_r = \frac{1}{\frac{1}{12}}$$
 of the mass of an atom of  $^{12}$ C

Relative atomic masses are used for atoms of elements.

## Relative molecular mass (M)

- Relative molecular mass  $(M_r)$  of an element or compound is the average mass of a molecule (or group of ions) of that element or compound relative to  $\frac{1}{12}$ th the mass of a 12**C**
- Relative molecular masses are used for molecules of both elements and compounds.

**Example:** what is the relative molecular mass of carbon dioxide,  $CO_2$ ?

$$Mr = 12.0 + (2 \times 16.0)$$
  
= 44.0

## Relative formula mass $(M_i)$

The relative formula mass is the sum of the relative atomic masses of all the atoms shown in the formula.

**Example:** what is the relative formula mass of CuSO<sub>4</sub>.5H<sub>2</sub>O?

$$63.5 + 32.1 + 4(16) + 5(18) = 249.6$$

## Relative molar mass (M)

Molar mass is the mass per mole of any substance (molecular or ionic).

Amount in moles = 
$$\frac{mass\ of\ substance\ in\ g}{molar\ mass\ in\ gmol-1}$$

## Avogadro constant (L)

- It is the number of particles (atoms, molecules or ions) in one mole of any substance.
- It is  $6.02 \times 10^{23}$

### Example:

 $6.02 \times 10^{23}$  helium atoms in 4.0g of He

 $6.02 \times 10^{23}$  carbon dioxide molecules in 44.0g of CO<sub>2</sub>

 $6.02 \times 10^{23}$  nitrate ions in 62.0g of NO<sub>3</sub>

No of particles = amount of substance (in mol) X Avogadro's constant No of ions = moles x Avogadro constant x number of those ions in the formula

## Worked example: 1

How many H<sub>2</sub>O molecules are there in 1.25g of water?

$$n = 1.25$$

$$= 0.0694 \text{ mol}$$

Number of molecules = 
$$6.02 \times 10^{23} \times 0.0694$$
  
=  $4.18 \times 10^{22}$ 

## Worked example: 2

Calculate the number of atoms in 0.0100mol of carbon dioxide, CO<sub>2</sub>?

1 mole of carbon dioxide =  $3 \times 6.02 \times 10^{23}$  atoms

0.0100 mol carbon dioxide = x

 $X = 0.01 \times 3 \times 6.02 \times 10^{23} = 1.81 \times 10^{22}$  atoms.

### **CHECKPOINT 6**

1. What is the mass of 100 million atoms of gold?

2. Calculate the number of atoms in 0.0100mol of carbon dioxide, CO<sub>2</sub>.

3. How many chloride ions are there in a 25.0 cm<sup>3</sup> of a solution of magnesium chloride of concentration  $0.400 \text{ moldm}^{-3}$ ?

4.	Malachite is an important mineral with formula $Cu_2CO_3(OH)_2$ . Calculate its relati
	formula mass.
5.	How many molecules of sugar ( $C_{12}H_{22}O_{11}$ ) are there in a teaspoon measure (4.20g
6.	Which contains more molecules: 10.0 grams of $O_2$ or 50.0 grams of iodine, $I_2$ ?

## **CALCULATING AMOUNTS OF CHEMICALS**

### Mole

It is the amount of substance that contains the same number of particles as the number of atoms in exactly 12g of  $^{12}\text{C}$ 

**Amount of substance in moles** = 
$$\frac{\text{mass in grams}}{\text{molar mass}}$$

### **WORKED EXAMPLE 1**:

Calculate the moles of NaCl in 2.2g of sodium chloride.

Molar mass of NaCl = 
$$23+35.5 = 58.5$$
  
Moles =  $\frac{2.2}{58.5} = 0.0376$  mol

You should be able to calculate molar mass of a compound from the atomic masses given in the period table

## **CHECKPOINT 7**

- 1. Calculate the number of moles of
- a) 13.76 g of (NH4)2SO4

b) 50.9 g of CuSO4.5H2O

- 2. Calculate the mass in grams for the following
- a) 0.70 moles of NaNO3

b) 0.12 moles of Al<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>

3.	How many particles are there of the specified substance?
	a) Atoms in 2.00g of sulfur, S
	b) Molecules in 4.00g of sulfur dioxide, SO <sub>2</sub>
	c) ions in 8.00g of sulfate ions, $SO_4^{2-}$

## CALCULATIONS USING REACTING MASSES

- A balanced equation for a reaction shows the same number of each species (atoms, molecules, ions or electrons) on both sides of the equation.
- It is also balanced for the masses of each species.
- This means that we can make predictions about the masses of reactants, which are needed to form a specified mass or amount of a product or the other way round.

## **Calculating reacting masses from equations**

### Worked example:

The equation for a reaction is:

$$SO_3 + H_2O \rightarrow H_2SO_4$$

What mass of sulfur tri oxide is needed to form 75.0g of sulfuric acid?

**Step 1**: calculate the molar masses of all substances you are told about and asked about, in this case, sulfurtrioxide and sulfuric acid.

$$M(SO_3) = 80.1 \text{ gmol}^{-1} \text{ and } M(H_2SO_4) = 98.1 \text{ gmol}^{-1}$$

Step 2: calculate the amount of sulfuric acid

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

$$= \frac{75.0}{98.1} = 0.765 \text{ mol}$$

**Step 3**: use the reaction ratio in the equation to work out the amount of sulfur trioxide needed

As the ratio is 1:1, the amount is the same, so  $n(SO_3) = 0.765$  mol

Step 4: Calculate the mass of sulfur trioxide

$$m = n \times M$$
  
= 0.765 \times 80.1  
= 61.2g

## Working out formulae and equations from reacting masses

### Worked example:

A 16.7g sample of a hydrate of sodium carbonate (Na<sub>2</sub>CO<sub>3</sub>.10H<sub>2</sub>O) is heated at a constant temperature for a specified time until the reaction is complete.

A mass of 3.15g of water is obtained. What is the equation for the reaction occuuring?

Step 1: calculate the molar masses of the relevant substances you are told about and asked about, in this case, sulfurtrioxide and sulfuric acid.

 $M(Na_2CO_3.10H_2O) = 286.1 \text{ gmol}^{-1}$ 

And  $M(H_2O)=18.0 \text{ gmol}^{-1}$ 

**Step 2**: calculate the amount of these substances

$$Na_2CO_3.10H_2O$$
  $n = \frac{m}{M} = \frac{16.7}{286.1} = 0.0584 \text{ mol}$ 

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

$$=\frac{16.7}{286.1}$$

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

$$=\frac{3.15}{18.0}$$

$$n = \frac{m}{M}$$
 =  $\frac{3.15}{18.0}$  = 0.175 mol

**Step 3**: use these amounts to calculate the simplest whole-number ratio for these substances.

 $Na_2CO_3.10H_2O$  and  $H_2O$  are in the ratio 0.0584 : 0.175 or 1:3

**Step 4:** use the ratio to work out the equation for the reaction

 $Na_2CO_3.10H_2O \rightarrow Na_2CO_3.7H_2O + 3H_2O$ 

We have worked out the Na<sub>2</sub>CO<sub>3</sub>.7H<sub>2</sub>O formula by considering the ratio of the two formulae.

#### **CHECKPOINT 8**

1. the equation for a reaction is

 $2NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$ 

What mass of ammonia is needed to form 100g of ammonium sulfate?

2. An oxide of copper is heated in a stream of hydrogen to constant mass. The masses of copper and water formed are Cu = 17.6g and  $H_2O = 2.56g$ . What is the equation for the reaction occurring?

3. A fertiliser manufacturer makes a batch of 20kg of ammonium nitrate. What mass of ammonia, in kg, does the manufacturer need to start with? 4. A sample of an oxide of iron was reduced to iron by heating with hydrogen. The mass of iron obtained was 4.35g and the mass of water was 1.86g. Deduce the equation for the reaction that occurred.

## THE YIELD OF A REACTION

In the laboratory, when you are making a product, you naturally want to obtain as much of it as possible from the reactants you start with. In industry, where the reactions occur on a much larger scale, and there is economic competition between the manufacturer, it is even more important to maximise the product of a reaction.

**Theoretical yield**: the maximum possible mass of a product in a reaction, assuming complete reaction and no losses

Actual yield: the actual mass obtained in a reaction

**Percentage yield:** the actual yield divided by the theoretical yield.

$$percentage\ yield = \frac{actual\ yield}{theoretical\ yield}\ x\ 100\%$$

**Learning tip:**  $1 \text{ kg} = 1 \times 10^3 \text{ g}$   $1 \text{ tonne} = 1 \times 10^6 \text{ g}$ 

### Worked example:

Iron(III) oxide reacts with carbon monoxide according to the equation:

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

When 25g of  $Fe_2O_3$  was reacted 10g of Fe is produced. What is the theoretical yield? And what percentage yield was achieved?

• Step 1: work out amount in mol of Iron oxide

• **Step 2:** use balanced equation to give moles of Fe

 $1 \text{ moles Fe}_2O_3: 2 \text{ moles Fe}$  So  $0.1566 \text{ Fe}_2O_3: 0.313 \text{moles Fe}$ 

• Step 3: work out mass of Fe

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

= 57.2%

### **CHECKPOINT 9**

1. Copper (ii) carbonate is decomposed to obtain copper(ii)oxide. The equation for the reaction is:

 $CuCO_3 \rightarrow CuO + CO_2$ 

What is the theoretical yield of copper(ii)oxide obtainable from 5.78g of copper(ii)carbonate?

2. Magnesium phosphate can be prepared from magnesium by reacting it with phosphoric acid.

The equation for the reaction is:

 $3Mg + 2H_3PO_4 \rightarrow Mg_3(PO_4)_2 + 3H_2$ 

3. A manufacture uses this reaction to obtain methanol from carbon monoxide and hydrogen:

$$CO + 2H_2 \rightarrow CH_3OH$$

The manufacturer obtains 4.07 tonnes of methanol starting from 4.32 tonnes of carbon monoxide

What is the percentage yield?

4. A student prepares a sample of copper(ii)sulfate crystals, CuSO<sub>4</sub>.5H<sub>2</sub>O, weighing 7.85g. She started with 4.68g copper(ii)oxide. What is the percentage yield?

5. a manufacturer makes some ethanoic acid using this reaction:

$$CH_3OH + CO \rightarrow CH_3COOH$$

Starting with 50.0kg of methanol, the manufacturer obtains 89.2kg of ethanoic acid. What is the percentage yield?

## LIMITING REAGENT

When a reaction is carried out in the laboratory, the reactants are not always present in the exact stoichiometric ratio determined by the equation. As a result, one reactant is used completely; some of the other reactant is left over. The reagent left over is called said to be in **excess**; the one used completely is said to be the **limiting reagent**.

A limiting reagent is the substance that determines the theoretical yield of product in a reaction.

- **Step 1:** calculate the amount (in moles) of one reagent and use the reaction stoichiometry to calculate the amount (in moles) of product that could be formed from this reagent.
- Step 2: calculate the amount (in moles) of the second reagent and use the reaction stoichiometry to calculate the amount (in moles) of product that could be formed from this second reagent.
- **Step 3:** the reagent that produces the least amount (in moles) of product is the limiting reagent.
- Step 4: calculate the theoretical yield of the product from the least amount (in moles) of product calculated in steps 1 and 2 (i.e. from the limiting reagent)

### Worked Example: 1

Solutions containing 12.8g of sulfuric acid (molar mass  $98.1 \text{gmol}^{-1}$ ) and 10.0g of sodium hydroxide (molar mass  $40.0 \text{gmol}^{-1}$ ) are mixed and produce sodium sulfate and water according to the following equation:

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

Calculate the mass of sodium sulfate (molar mass 142.1gmol $^{-1}$ ) produced.

**Step 1:** amount of NaOH = 
$$\frac{mass}{molar\ mass} = \frac{10.0}{40.0} = 0.250\ mol$$

Ratio of  $Na_2SO_4$  to NaOH = 1:2

Theoretical amount of Na<sub>2</sub>SO<sub>4</sub> produced =  $\frac{1}{2}$  x 0.250 = 0.125 mol

**Step 2:** amount of 
$$H_2SO_4 = \frac{mass}{molar\ mass} = \frac{12.8}{98.1} = 0.130\ mol$$

Ratio of  $Na_2SO_4$  to  $H_2SO_4 = 1:1$ 

Theoretical amount of  $Na_2SO_4$  produced = 0.130 mol

**Step 3:** the reagent that produces the least product (0.125 mol) is sodium hydroxide, so this is the limiting reagent.

$$= 0.125 \times 142.1$$

$$= 17.8 g$$

## **ATOM ECONOMY**

- Atom economy is a measure of the amount of starting materials that end up as useful products
- It is not the same as the **yield**.
- Atom economy is calculated using the balanced chemical equation for the reaction, assuming it produces 100% yield.

Atom economy = 
$$\frac{molar\ mass\ of\ the\ desired\ product}{sum\ of\ the\ molar\ mass\ of\ all\ the\ products}$$
 × 100

- A reaction with high atom economy makes use of most of the atoms of the reactants, with few wasted as by-products.
- This reduces the amount of waste products a company has to deal with, which in turn reduces the cost of waste treatment.
- Atom economy can be improved by finding uses for any by-products.
- Sustainable chemistry requires chemists to design processes with high atom economy that minimise production of waste products.

## Worked example:

Calculate the percentage atom economy of using copper oxide and sulfuric acid to make copper sulfate in solution:

$$CuO(s) + H_2SO_4(aq) \rightarrow CuSO_4(aq) + H_2O(l)$$

Atom economy = 
$$\frac{mass\ of\ copper\ sulfate}{mass\ of\ copper\ oxide+sulfuric\ acid} \times 100$$

$$= \frac{63.5+32.0+(4\times16)}{(63.5+16.0)+(2+32.0+4\times16))} \times 100 = 89.9\%$$

### **CHECKPOINT 10**

- 1. Calculate the percentage atom economy of the **named product** in the reactions shown below:
  - a) hydrogen in the reaction  $Zn + 2HCl \rightarrow ZnCl_2 + H_2$
  - **b) iron** in the reaction  $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$
  - c) calcium oxide in the reaction  $CaCO_3 \rightarrow CaO + CO_2$

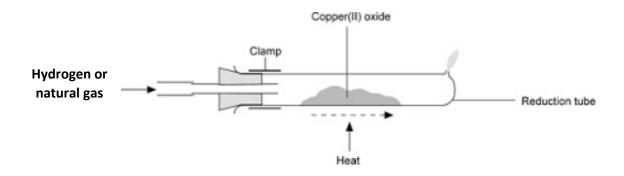
## **EMPIRICAL FORMULAE**

- The **empirical formula** is the simplest whole number ratio of the atoms of each element in a compound.
- The term "empirical" indicates that some information has been found by experiment.

### One example of an experimental method

- A simple example involves determining the formula of an oxide of copper. This oxide can be converted to copper by removing the oxygen.
  - Here are the steps in the experiment.
- 1. Place a known mass of the oxide of copper in the tube.
- 2. Heat the oxide in a stream of hydrogen gas (or natural gas, which is mostly methane)
- 3. The gas reacts with oxygen in the copper oxide and forms steam
- 4. The colour of the solid gradually changes to orange brown which is the colour of copper.
- 5. The excess gas is burned off at the end of the tube for safety reasons.
- 6. After cooling, remove and weigh the solid copper.
- 7. It is good practice to heat the solid again in the stream of the gas to check whether its mass changes.

Heating to a constant mass suggests that the conversion to copper is complete.



### **Calculating empirical formulae**

The calculation method involves these steps.

- 1. Divide the mass, or percentage composition by mass of each element by its relative atomic mass.
- 2. If the necessary, divide the answers from this step by the smallest of the numbers.
- 3. This gives numbers that should be in an obvious whole number ratio, such as 1:2 or 3:2
- 4. These whole numbers are used to write the empirical formula.

It may help you to organise the calculation using a table, although this is not essential.

### **Calculation using masses**

Assume that these are the results of the experiment outlined on the left.

Mass of copper oxide = 4.28g

Mass of copper = 3.43g

Mass of oxygen removed is 4.28 - 3.43 = 0.85g

**Table A** is the calculation table for these results

	Cu	0
Mass of element /g	3.43	0.85
Relative Atomic mass	63.5	16.0
Division by A <sub>r</sub>	0.0540	0.0531
Ratio	1	1

The ratio is obviously 1:1, so the empirical formula is CuO

## Calculation using percentage composition

You do the calculation in the same way, except that you divide percentages instead of masses by the relative atomic mass.

The calculation table, table B refers to a compound containing three elements. The compound has the percentage composition by mass C=38.4%, H=4.8%, Cl=56.8%

	С	Н	Cl
% of element	38.4	4.8	56.8
Relative Atomic mass	12.0	1.0	35.5
Division by A <sub>r</sub>	3.2	4.8	1.6
Ratio	2	3	1

You can see that the empirical formula is  $C_2H_3Cl$ 

## Calculation when the oxygen value is not provided

A compound has the percentage composition by mass Na=29.1%, S=40.5%, with the remainder being oxygen.

The percentage of oxygen = 
$$100 - (29.1 + 40.5)$$
  
=  $30.4\%$ 

Table C is the calculation table

	Na	S	0
% of element	29.1	40.5	30.4
Relative Atomic mass	23.0	32.1	16.0
Division by $A_{ m r}$	1.27	1.26	1.90
Division by the smallest	1	1	1.5
Ratio	2	2	3

You can see that the empirical formula is  $Na_2S_2O_3$ 

## **Calculation using combustion analysis**

1.87g sample of an organic compound was completely burned, forming 2.65g of carbondioxide and 1.63g water.

In this type of calculation, the first steps are to calculate the masses of carbon and hydrogen in the carbondioxide and water.

- The relative molecular mass of carbondioxide is 44.0 but, because the relative atomic mass of carbon is 12, the proportion of carbon in carbondioxide is always  $12.0 \div 44.0$
- Similarly, the proportion of hydrogen in water is always  $(2 \times 1.0) \div 18.0$

All of the carbon in the carbondioxide comes from the carbon in the organic compound. Similarly, all of the hydrogen in eater comes from the hydrogen in the organic compound. In this example:

Mass of carbondioxide = 
$$\frac{2.65 \times 12.0}{44.0}$$
 = 0.723g

Mass of hydrogen = 
$$\frac{1.63 \times 2.0}{18.0}$$
 = 0.181g

These two masses add up to 0.904g

The original mass of the organic compound was 1.87g, so the difference must be the mass of oxygen present in the organic compound.

The mass of oxygen = 
$$1.87 - 0.904 = 0.966g$$

Table D is the calculation table. You can see that the empirical formula of the sample compound is  $\text{CH}_3\text{O}$ 

	С	Н	0
Mass of element /g	0.723	0.181	0.966
Relative Atomic mass	12.0	1.0	16.0
Division by $A_{\rm r}$	0.0603	0.181	0.0604
Ratio	1	3	1

#### **EXAM HINT**

Take care to look out for decimals that indicate obvious fraction, e.g., simple ratio 1:1.33 indicates an empirical formula of 3:4. How would a ratio of 1:1.25 convert into an empirical formula?

#### **LEARNING TIP**

Divide by the relative atomic mass, not the atomic number or the relative molecular mass.

For oxygen, only divide by 16.0 not by 8 or 32.

#### CHECKPOINT 11

1. A compound has the percentage composition by mass Ca = 24.4%, N = 17.1% and O = 58.5%, What is its empirical formula?

2. Combustion analysis of 2.16g of an organic compound produced 4.33g of carbondioxide and 1.77g of water. What is its empirical formula?

## **MOLECULAR FORMULAE**

• Molecular formula is the actual number of atoms of each element in a molecule.

• Sometimes the empirical formula of a compound is the same as its molecular formula.

**Example**: water, H<sub>2</sub>O

Examples of compounds with different empirical and molecular formulae:

*Hydrogen peroxide*: empirical formula: HO Molecular formula:  $H_2O_2$ 

**Butane** empirical formula:  $C_2H_5$  Molecular formula:  $C_4H_{10}$ 

#### Worked example: 1

In this example, the empirical formula is given

A compound has the empirical formula CH and a relative formula mass of 104

The formula mass of the empirical formula is 13.0

 $104 \div 13.0 = 8$ , so the molecular formula of the compound is  $C_8H_8$ 

### Worked example: 2

In this example, you first have to work out the empirical formula. A compound contains the percentage composition by mass Na = 34.3%, C = 17.9%, O = 47.8%, and has a molar mass of  $134 \text{ gmol}^{-1}$ . The calculations are shown below.

	Na	С	0
Mass of element /g	34.3	17.9	47.8
Relative Atomic mass	23.0	12.0	16.0
Division by $A_{\rm r}$	1.49	1.49	2.99
Ratio	1	1	2

The empirical formula is  $NaCO_2$ 

The formula mass of the empirical formula is  $23.0 + 12.0 + (2 \times 16.0) = 67.0$ 

The molar mass, 134 is 2 x 67.0, so the molecular formula of the compound is  $Na_2C_2O_4$ 

# THE IDEAL GAS EQUATION pV = nRT

This can be used for gases (or volatile liquids above their boiling temperatures) to find the amount of a substance in moles.

If the mass of the substance is also known, then the molar mass of the substance can be calculated.

This gives the extra information needed to work out a molecular formula from an empirical formula.

#### SI units

p = pressure in Pascals (Pa)

V = volume in cubic meters (m<sup>3</sup>)

T = temperature in kelvins (K)

n = amount of substance in moles

 $R = the gas constant. (8.13 J mol^{-1})$ 

CONVERSION	HOW TO DO IT
kPa → Pa	Multiply by 10 <sup>3</sup>
$Cm^3 \rightarrow m^3$	Divide by 10 <sup>6</sup>
$dm^3 \rightarrow m^3$	Divide by 10 <sup>3</sup>
°C → K	Add 273

### Worked example: 1

0.280 g sample of a gas has a volume of 58.5cm³, measured at a pressure of 120kPa and a temperature of 70°C. Calculate the molar mass of the gas.

$$p = 120 \text{ kPa}$$
 =  $120 \text{x} 10^3 \text{ Pa}$ 

$$V = 58.5 \text{ cm}^3 = 58.5 \text{ x } 10^{-6} \text{ m}^3$$

$$T = 70 \, ^{\circ}C = 343 \, \text{K}$$

$$R = 8.13 \text{ J mol}^{-1} \text{ K}$$

$$n = \frac{pV}{RT} = \frac{120 \times 10^3 \times 58.5 \times 10^{-6}}{8.31 \times 343} = 0.00246 \text{ mol}$$

$$M = \frac{m}{n}$$
 =  $\frac{0.280}{0.00246}$  = 114 g mol<sup>-1</sup>

**1.** A compound has the percentage composition by mass C = 52.2%, H = 13.0%, O = 10.0%34.8%. A sample containing 0.173g of the compound had a volume of 95.0cm3 when measured at 105kPa and 45°C.

What is the molecular formula of this compound?

2. A 2.82 g sample of a gas has a volume of 1.26dm³, measured at a pressure of 103 kPa and a temperature of 55°C. Calculate the molar mass of the gas.

3.	A compound has the percentage by composition by mass $C=40.0\%$ , $H=6.7\%$ $O=53.3\%$ . A sample containing 0.146g of the compound had a volume of 69.5cm.
	when measured at 98kPa and 63°C. What is the molecular formula of this compound?

## **MOLAR VOLUME CALCULATIONS**

Molar volume is the volume occupied by 1 mol of any gas; this is normally 24dm<sup>3</sup> or  $24000cm^3$  at r.t.p

$$V_{\rm m}$$
 = 24 dm<sup>3</sup> mol<sup>-1</sup> at rtp  $or$   $V_{\rm m}$  = 24 000 cm<sup>3</sup> mol<sup>-1</sup> at rtp

# Calculations using molar volume

Amount of gas (in moles) = 
$$\frac{\text{volume in dm3}}{\text{molar volume(24)}}$$

Or

Amount of gas (in moles) = 
$$\frac{\text{volume in cm3}}{\text{molar volume}(24\,000)}$$

1. A piece of magnesium with a mass of 1.00g is added to an excess of dilute hydrochloric acid. What volume of hydrogen gas is formed?

2. Calcium carbonate reacts with nitric acid to form calcium nitrate, water and carbondioxide, as shown in the equation.

$$CaCO_3(s) + 2HNO_3(aq) \rightarrow Ca(NO_3)_2(aq) + H_2O(l) + CO_2(g)$$

In a reaction, 100cm³ of carbondioxide is formed. What mass of calcium carbonate is needed for this?

3.	Ammonium sulfate reacts with sodium hydroxide to form sodium sulfate and ammonia.  What volume of ammonia is formed by reacting 2.16g of ammonium sulfate with excess sodium hydroxide solution?
4.	10.0 g of copper(ii)oxide is heated with hydrogen according to the equation    CuO(s) + H₂(g) → Cu(s) + H₂O(l)  What volume of hydrogen gas is needed to react with the copper (ii) oxide and what mass of copper is formed

## **CONCENTRATIONS OF SOLUTIONS**

# Calculations using mass concentration (g dm<sup>-3</sup>)

Mass concentration in 
$$g \, dm^{-3} = \frac{mass \, of \, solute \, in \, g}{volume \, of \, solution \, in \, dm^3}$$

Worked example:

200 cm<sup>3</sup> of a solution contains 5.68g of sodium bromide. What is its mass concentration?

Mass concentration = 
$$\frac{m}{V}$$
 =  $\frac{5.68}{0.200}$  = 28.4 g dm<sup>-3</sup>

# Calculations using molar concentration (mol dm<sup>-3</sup>)

- It is used to be called molarity.
- It is used more often than mass concentration
- If only the term 'concentration' is mentioned, then you should assume that it refers to molar concentration.

$$Molar concentration = \frac{amount}{volume}$$

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

#### Worked example:

A chemist makes 500 cm<sup>3</sup> of a solution of nitric acid of concentration 0.800 mol dm<sup>-3</sup>. What mass of  $HNO_3$  does she need?

Step 1: you are given values of V and C, so you can use the second expression to calculate a value for n

 $n = C \times V$ 

 $= 0.800 \times 0.500$ 

 $= 0.400 \ mol$ 

Step 2: You can now use the first expression to calculate the mass of nitric acid

 $m = n \times M$ 

 $= 0.400 \times 63.0$ 

= 25.2 g

## Calculations from equations using concentration and mass

In this type of calculations, you can use an equation to calculate the mass of a reactant or product if you are given the volume and molar concentration of another substance, and vice versa.

### Worked example:

An excess of magnesium is added to 100cm<sup>3</sup> of 1.50 mol dm<sup>-3</sup> hydrochloric acid. The equation for the reaction is:

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

What mass of hydrogen is formed?

Step 1: you are given values of V and C, so you can use the second expression to calculate a value for n for hydrochloric acid.

$$n = C \times V$$

$$= 0.100 \times 1.50 = 0.150 \text{ mol}$$

Step 2: the ratio for HCl:  $H_2$  is 2:1, so  $n(H_2) = 0.150 \div 2 = 0.0750$  mol

Step 3: You can now use the first expression to calculate the mass of nitric acid

$$m = n \times M$$

$$= 0.0750 \times 2.0 = 0.15 g$$

1. 50.0g of sodium hydroxide is dissolved in water to make 1.50 dm³ of solution. What is the molar concentration of the solution.

2. 150cm³ of 0.125 mol dm⁻³ lead(ii)nitrate solution is mixed with an excess of potassium iodide solution. The equation for the reaction occurs is:  $Pb(NO_3)_2(aq) + 2KI(aq) \rightarrow PbI_2(s) + 2KNO_3(aq)$ 

## **CONCENTRATIONS IN PPM**

**Parts per million (ppm)**: the number of parts of one substance in one million parts of another substance; a measure used to describe chemical concentration; usually, 'parts' refers to masses of both substances, or to volumes of both substances.

#### **Calculations for solutions in PPM**

A concentration of 1 ppm means 1g in 1000 000g, or 1 mg in 1000 000 mg

Concentration in ppm = 
$$\frac{mass\ of\ solute\ \times 1000\ 000}{mass\ of\ solvent}$$

#### Worked example: 1

A solution contains 0.176g of solute dissolved in 750g of solvent. What is the concentration in ppm?

As the units of solute and solvent are the same, the values can be directly inserted into the expression

Concentration in ppm = 
$$\frac{mass \ of \ solute \ in \times 1000 \ 000}{mass \ of \ solvent}$$
$$= \frac{0.176 \times 1000 \ 000}{750}$$
$$= 235 \ ppm$$

#### Worked example: 2

A mass of 23mg of sodium chloride is dissolved in 900g of water. What is the concentration of sodium chloride in the solution in ppm?

As the units of solute and solvent are different, either the mass of solute or the mass of solvent must be converted so they are the same. Then the values can be directly inserted into the expression.

First convert the mass of sodium chloride from mg to g(divide by 1000)

Mass of sodium chloride =  $23 \div 1000 = 0.023g$ 

Concentration in ppm = 
$$\frac{mass \ of \ solute \ in \times 1000 \ 000}{mass \ of \ solvent}$$
$$= \frac{0.023 \times 1000 \ 000}{900}$$
$$= 26 \ ppm$$

# **Calculations for gases in PPM**

This expression can be used to calculate concentrations in ppm.

Concentration in ppm = 
$$\frac{volume\ of\ gas \times 1000\ 000}{volume\ of\ air}$$

The volumes can be in any units, but they must be the same units. If different units are given, then one of them must be converted.

#### Worked example: 1

Some nitrogen dioxide gas, with a volume of 1.5 dm³, mixes with 10 000 dm³ of air. What is the concentration of nitrogen dioxide, in ppm, in the air?

As the volume units of both gases are the same, then the values can be directly inserted into the expression.

Concentration in ppm = 
$$\frac{volume \ of \ gas \times 1000 \ 000}{volume \ of \ air}$$
$$= \frac{1.5 \times 1000 \ 000}{900}$$
$$= 150 \ ppm$$

#### Worked example: 2

Two samples of air containing sulfur dioxide were analysed. The results for Sample 1 showed that 500dm<sup>3</sup> of air contained 37cm<sup>3</sup>.

### Sample 1:

Concentration in ppm = 
$$\frac{volume \ of \ gas \times 1000 \ 000}{volume \ of \ air}$$
$$= \frac{37 \div 1000 \times 1000 \ 000}{500}$$
$$= 74 \ ppm$$

### Sample 2:

Concentration in ppm = 
$$\frac{volume \ of \ gas \times 1000 \ 000}{volume \ of \ air}$$
$$= \frac{1.4 \times 1000 \ 000}{4000}$$
$$= 350 \ ppm$$

Sample 2 has the higher concentration

1. 0.2g of potassium sulfate is dissolved in water to make 800g of solution. What is the concentration of the salt in ppm?

2. 200dm³ of air contains 58cm³ of chlorine. What is the concentration of chlorine in ppm?

3. A solution of lead sulfate (PbSO<sub>4</sub>) contains 0.425 g of lead sulfate in 100.0 g of water. What is this concentration in ppm?

4. Helium gas, 3.0 x 10<sup>-4</sup> g, is dissolved in 200 g of water. Express this concentration in parts per million.

5.	A 900.0 g sample of sea water is found to contain 6.7 x $10^{-3}$ g Zn. Express this
	concentration in ppm.
6.	A solution has a concentration of 0.033g/kg. What is its concentration in ppm?

**1.** What mass of barium sulfate would be produced from 10 g of barium chloride in the following reaction?

 $BaCl_2 + H_2SO_4 \rightarrow BaSO_4 + 2HCl$ 

**2.** What volume of ammonia gas would be needed to produce 40 g of ammonium nitrate in the following reaction?

 $NH3(g) + HNO3(aq) \rightarrow NH4NO3(aq)$ 

**3.** In the reaction between calcium carbonate and nitric acid what mass of calcium nitrate and what volume of carbon dioxide would be produced from 33.3 g of calcium carbonate?

Calculate the concentration of sodium hydroxide if  $25~\mathrm{cm}^3$  of sodium hydroxide reacts with  $21.0 \text{ cm}^3$  of  $0.2 \text{ mol dm}^{-3}$  HCl

Calculate the concentration of hydrochloric acid if  $20~\mathrm{cm^3}$  of hydrochloric acid *5.* reacts with 20.0 cm $^3$  of a solution of NaOH containing 40 g dm $^{-3}$  of NaOH

## **SALT PREPARATION**

Salts are ionic compounds. The positive ion or cation is usually a metal ion or an ammonium ion,  $NH_4^+$ . The negative ion, or anion, comes from an acid such as  $SO_4^{2-}$  in  $H_2SO_4$ .

- ➤ **A double salt c**ontains more than one cation or anion. They form when a solution of two simple salts crystallises to form a single substance.
- ➤ Salts can be produced by neutralising acids with an alkali, carbonate or metal oxide or hydroxide.
- > Salts can be produced by reacting acids with reactive metals.
- ➤ A soluble salt must be crystallised from a saturated solution- concentrate the solution by driving off some of the water, leaving to evaporate and then filtering.
- ➤ An insoluble salt forms a precipitate and can be filtered off, washed and dried.

### METHOD FOR PREPARING A SOLUBLE SALT

#### If using an insoluble base, metal or solid carbonate

#### Procedure:

- 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 a 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.

#### Method for preparing an insoluble salt

- Insoluble salts can be made by mixing appropriate solutions of ions so that a
   precipitate is formed.
- 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

#### Preparation of double salt

#### Ammonium iron(II) sulfate, or Mohr's Salt,

- ❖ Ammonium iron(II) sulfate, or Mohr's Salt, is the inorganic compound with the formula  $(NH_4)_2Fe(SO_4)_2\cdot 6H_2O$ . Containing two different cations,  $Fe^{2+}$  and  $NH_4^+$ ,
- It is classified as a double salt of ferrous sulfate and ammonium sulfate
- Mohr's salt is prepared by dissolving an equimolar mixture of hydrated ferrous sulfate and ammonium sulfate in water containing a little sulfuric acid, and then subjecting the resulting solution to crystallization. Ferrous ammonium sulfate forms light green crystals.