2.1.3 Amount 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 x 3 = 100.1

**molar gas volume** (gas volume per mole, units dm$^3$ mol$^{-1}$). This is the volume of 1 mole of a gas at a given temperature and pressure. All gases have this same volume. At room pressure (1 atm) and room temperature 25°C the molar gas volume is 24 dm$^3$ mol$^{-1}$

Avogadro’s Constant

There are 6.02 x $10^{23}$ atoms in 12 grams of carbon-12. Therefore explained in simpler terms ‘One mole of any specified entity contains 6.02 x $10^{23}$ of that entity’:

Avogadro’s Constant can be used for atoms, molecules and ions

1 mole of copper atoms will contain 6.02 x $10^{23}$ atoms
1 mole of carbon dioxide molecules will contain 6.02 x $10^{23}$ molecules
1 mole of sodium ions will contain 6.02 x $10^{23}$ ions

For pure solids, liquids and gases

\[
\text{amount} = \frac{\text{mass}}{\text{Mr}}
\]

Unit of Mass: grams
Unit of amount: mol

Many questions will involve changes of units

1000 mg = 1g
1000 g = 1kg
1000 kg = 1 tonne

**Example 1:** What is the amount, in mol, in 35.0g of CuSO$_4$?

\[
\text{amount} = \frac{\text{mass}}{\text{Mr}}
\]

\[
= \frac{35}{(63.5 + 32 + 16 \times 4)}
\]

\[
= 0.219 \text{ mol}
\]

**Example 2:** What is the amount, in mol, in 75.0mg of CaSO$_4$.2H$_2$O?

\[
\text{amount} = \frac{\text{mass}}{\text{Mr}}
\]

\[
= \frac{0.075}{(40 + 32.0 + 16.0 \times 4 + 18.0 \times 2)}
\]

\[
= 4.36 \times 10^{-4} \text{ mol}
\]

**Significant Figures**

Give your answers to the same number of significant figures as the number of significant figures for the data you given in a question. If you are given a mixture of different significant figures, use the smallest
Empirical formulae

**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.

**Example 3:** Calculate the empirical formula for a compound that contains 1.82g of K, 5.93g of I and 2.24g of O

Step 1: Calculate amount, in mol, by dividing each mass by the atomic mass of the element
K = 1.82 / 39.1 = 0.0465 mol
I = 5.93/126.9 = 0.0467 mol
O = 2.24/16 = 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 = 1
I = 0.0467 / 0.0465 = 1
O = 0.14 / 0.0465 = 3

Empirical formula = KI\textsubscript{3}O\textsubscript{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 4:** work out the molecular formula for the compound with an empirical formula of C\textsubscript{3}H\textsubscript{6}O and a M\textsubscript{r} of 116

C\textsubscript{3}H\textsubscript{6}O has a mass of 58
The empirical formula fits twice into M\textsubscript{r} of 116

So molecular formula is C\textsubscript{6}H\textsubscript{12}O\textsubscript{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.
The water of crystallisation in calcium sulphate crystals can be removed as water vapour by heating as shown in the following equation.

\[ \text{CaSO}_4 \cdot x \text{H}_2\text{O}(s) \rightarrow \text{CaSO}_4(s) + x \text{H}_2\text{O}(g) \]

**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).

Small amounts of hydrated calcium sulphate, such as 0.100 g, should not be used in this experiment as errors in weighing are too high.

Large amounts of hydrated calcium sulphate, such as 50g, should not be used in this experiment as the decomposition is likely to be incomplete.

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 6.** 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 \( \text{ZnSO}_4 \cdot x\text{H}_2\text{O} \)

**Calculate the mass of \( \text{H}_2\text{O} \):**

\[ 3.51 \text{ g} - 1.97 \text{ g} = 1.54 \text{ g} \]

**Calculate moles of \( \text{ZnSO}_4 \):**

\[ \frac{1.97}{161.5} = 0.0122 \text{ mol} \]

**Calculate moles of \( \text{H}_2\text{O} \):**

\[ \frac{1.54}{18} = 0.085 \text{ mol} \]

**Calculate ratio of mole of \( \text{ZnSO}_4 \) to \( \text{H}_2\text{O} \):**

\[ \frac{0.0122}{0.0122} = 1 \]

\[ X = 7 \]
Concentration of Solutions

A solution is a mixture formed when a solute dissolves in a solvent. In chemistry we most commonly use water as the solvent to form aqueous solutions. The solute can be a solid, liquid or a gas.

Molar concentration can be measured for solutions. This is calculated by dividing the amount in moles of the solute by the volume of the solution. The volume is measured in dm$^3$. The unit of molar concentration is mol dm$^{-3}$; it can also be called molar using symbol M.

### Concentration = \( \frac{\text{amount}}{\text{volume}} \)

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

**Unit of Volume:** dm$^3$

### Converting volumes

- A m$^3$ is equivalent to a cube
  - 100cm x 100cm x 100cm = 1000000cm$^3$

- 1 m$^3$ = 1000 dm$^3$ or 1000L
- To convert m$^3$ into dm$^3$ multiply by 1000

- A cm$^3$ is equivalent to a cube
  - 1cm x 1cm x 1cm = 1000cm$^3$

- 1 cm$^3$ = 1 ml
- 1 dm$^3$ = 1000 cm$^3$ or 1000mL
- To convert cm$^3$ into dm$^3$ divide by 1000

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<tr>
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### Example 7
What is the concentration of solution made by dissolving 5.00g of Na$_2$CO$_3$ in 250 cm$^3$ water?

Amount = \( \frac{\text{mass}}{\text{Mr}} \)

= \( \frac{5}{(23.0 \times 2 + 12 + 16 \times 3)} \)

= 0.0472 mol

Concentration = \( \frac{\text{amount}}{\text{Volume}} \)

= \( \frac{0.0472}{0.25} \)

= 0.189 mol dm$^{-3}$

### Example 8
What is the concentration of solution made by dissolving 10kg of Na$_2$CO$_3$ in 0.50 m$^3$ water?

Amount = \( \frac{\text{mass}}{\text{Mr}} \)

= \( \frac{10000}{(23.0 \times 2 + 12 + 16 \times 3)} \)

= 94.2 mol

Concentration = \( \frac{\text{amount}}{\text{Volume}} \)

= \( \frac{94.2}{500} \)

= 0.19 mol dm$^{-3}$
Mass Concentration

The concentration of a solution can also be measured in terms of mass of solute per volume of solution

Mass Concentration = \( \text{mass} \over \text{volume} \)

Unit of mass concentration: g dm\(^{-3}\)
Unit of Mass g
Unit of Volume: dm\(^3\)

Ions dissociating

When soluble ionic solids dissolve in water they will dissociate into separate ions. This can lead to the concentration of ions differing from the concentration of the solute.

Example 9

If 5.86g (0.1 mol) of sodium chloride (NaCl) is dissolved in 1 dm\(^3\) of water then the concentration of sodium chloride solution would be 0.1moldm\(^{-3}\).

However the 0.1mol sodium chloride would split up and form 0.1 mol of sodium ions and and 0.1 mol of chloride ions. The concentration of sodium ions is therefore 0.1 mol dm\(^{-3}\) and the concentration of chloride ions is also 0.1 mol dm\(^{-3}\).

\[
\text{NaCl(s) +aq} \rightarrow \text{Na}^+(aq) + \text{Cl}^-(aq)
\]

0.1mol 0.1mol 0.1mol

Example 10

If 9.53g (0.1 mol) of magnesium chloride (MgCl\(_2\)) is dissolved in 1 dm\(^3\) of water then the concentration of magnesium chloride solution (MgCl\(_2\)aq) would be 0.1moldm\(^{-3}\).

However the 0.1mol magnesium chloride would split up and form 0.1 mol of magnesium ions and 0.2 mol of chloride ions. The concentration of magnesium ions is therefore 0.1 mol dm\(^{-3}\) and the concentration of chloride ions is now 0.2 mol dm\(^{-3}\).

\[
\text{MgCl}_2(s) +aq \rightarrow \text{Mg}^{2+}(aq) + 2\text{Cl}^-(aq)
\]

0.1mol 0.1mol 0.2mol

Making a solution

- Weigh the sample bottle containing the required mass of solid on a 2 dp balance
- Transfer to beaker and reweigh sample bottle
- Record the difference in mass

- Add 100cm\(^3\) of distilled water to the beaker. 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.

Alternatively the known mass of solid in the weighing bottle could be transferred to beaker, 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.
**Dilutions**

**Diluting a solution**

- Pipette 25cm\(^3\) of original solution into a 250cm\(^3\) 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.

Using a volumetric pipette is more accurate than a measuring cylinder because it has a smaller uncertainty.

Use a teat pipette to make up to the mark in volumetric flask to ensure volume of solution accurately measured and one doesn’t go over the line.

**Calculating Dilutions**

Diluting a solution will not change the amount of moles of solute present but increase the volume of solution and hence the concentration will lower

\[
\text{amount} = \text{volume} \times \text{concentration}
\]

If amount of moles does not change then

Original volume \(\times\) original concentration = new diluted volume \(\times\) new diluted concentration

so

\[
\text{new diluted concentration} = \frac{\text{original concentration} \times \text{Original volume}}{\text{new diluted volume}}
\]

The new diluted volume will be equal to the original volume of solution added + the volume of water added.

**Example 11**

If 50 cm\(^3\) of water are added to 150 cm\(^3\) of a 0.20 mol dm\(^{-3}\) NaOH solution, what will the concentration of the diluted solution be?

\[
\text{new diluted concentration} = \frac{0.20 \times 0.150}{0.200} = 0.15 \text{ mol dm}^{-3}
\]

**Example 12**

What volume of water in cm\(^3\) must be added to dilute 5.00 cm\(^3\) of 1.00 mol dm\(^{-3}\) hydrochloric acid so that it has a concentration of 0.050 mol dm\(^{-3}\) ?

Amount in mol original solution = conc \(\times\) vol

\[
= 1.00 \times 0.005 = 0.005
\]

New volume = amount /conc

\[
= 0.005/0.05 = 0.1 \text{dm}^3 = 100 \text{cm}^3
\]

Volume of water added = 100-5 = 95cm\(^3\)

**Safety and hazards**

- Irritant - dilute acid and alkalis - wear goggles
- 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.
Ideal Gas Equation

The ideal gas equation applies to all gases and mixtures of gases. If a mixture of gases is used the value n will be the total moles of all gases in the mixture.

The biggest problems students have with this equation is choosing and converting to the correct units, so pay close attention to the units.

Example 13: What is the mass of Cl₂ gas that has a pressure of 100kPa, temperature 20°C, volume 500cm³. (R = 8.31)

\[
\text{moles} = \frac{PV}{RT} = \frac{100000 \times 0.0005}{(8.31 \times 293)} = 0.0205 \text{ mol}
\]

Mass = amount x Mr
\[
= 0.0205 \times (35.5 \times 2)
= 1.46 \text{ g}
\]

Example 14: 0.150g of a volatile liquid was injected into a sealed gas syringe. The gas syringe was placed in an oven at 70°C at a pressure of 100kPa and a volume of 80cm³ was measured. What is the Mr of the volatile liquid? (R = 8.31)

\[
\text{moles} = \frac{PV}{RT} = \frac{100000 \times 0.00008}{(8.31 \times 343)} = 0.00281 \text{ mol}
\]

Mr = mass/amount
\[
= \frac{0.15}{0.00281}
= 53.4 \text{ g mol}^{-1}
\]

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 ideal gas equation \(PV = nRT\)

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.

Converting temperature

\(^{\circ}\text{C} \rightarrow \text{K add 273}\)

PV = nRT

Unit of Pressure (P): Pa
Unit of Volume (V): m³
Unit of Temp (T): K
n = moles
R = 8.31 J K⁻¹mol⁻¹
Example 15
40 cm$^3$ of oxygen and 60 cm$^3$ of carbon dioxide, each at 298 K and 100 kPa, were placed into an evacuated flask of volume 0.50 dm$^3$. What is the pressure of the gas mixture in the flask at 298 K?

There are two approaches to solving this
1. Work out amount in mol of gas using ideal gas equation then put back into ideal gas equation with new conditions
2. Or combine the equation $n = \frac{PV}{RT}$ as on right

\[
\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}
\]

Can do this as moles of gas do not change

As Temperature is the same can make the above equation $P_1V_1 = P_2V_2$

\[
P_2 = \frac{P_1V_1}{V_2} = \frac{100000 \times 1 \times 10^{-4}}{5 \times 10^{-4}} = 20000 \text{Pa}
\]

Example 16: What is the volume in dm$^3$ at room temperature and pressure of 50.0g of Carbon dioxide gas?

\[
\text{amount} = \frac{\text{mass}}{M_r} = \frac{50}{12 + 16 \times 2} = 1.136 \text{ mol}
\]

Gas Volume (dm$^3$) = amount x 24

\[
= 1.136 \times 24 = 27.3 \text{ dm}^3 \text{ to 3 sig fig}
\]

Example 17: 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?

\[
\text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O(l)}
\]

1 mole 2 mole 1 mole

500cm$^3$ 1dm$^3$ 500cm$^3$

Simply multiply gas volume x2

Example 18: An important reaction which occurs in the catalytic converter of a car is

\[
2\text{CO}(g) + 2\text{NO}(g) \rightarrow 2\text{CO}_2(g) + \text{N}_2(g)
\]

In this reaction, when 500 cm$^3$ of NO reacts with 500 cm$^3$ of CO at 650 °C and at 1 atm. Calculate the total volume of gases produced at the same temperature and pressure?

\[
\text{total volume of gases produced} = 750 \text{cm}^3
\]
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 can be used for atoms, molecules and ions.

1 mole of copper atoms will contain $6.02 \times 10^{23}$ atoms  
1 mole of carbon dioxide molecules will contain $6.02 \times 10^{23}$ molecules  
1 mole of sodium ions will contain $6.02 \times 10^{23}$ ions

**No of particles = amount of substance (in mol) X Avogadro's constant**

**Example 19:** 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 $6.02 \times 10^{23}$  
= 0.05055 x $6.02 \times 10^{23}$  
= 3.04 x$10^{22}$

**Example 20:** 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 x 2  
= 0.0200  
Number ions of Cl$^-$ = amount x $6.02 \times 10^{23}$  
= 0.0200 x $6.02 \times 10^{23}$  
= 1.204 x$10^{22}$

**Example 21:** How many molecules of ethanol are there in a 0.500 dm$^3$ of ethanol (CH$_3$CH$_2$OH) liquid? The density of ethanol is 0.789 g cm$^{-3}$

Mass = density x Volume  
ethanol = 0.789 x 500  
= 394.5g  
amount = mass/Mr  
= 394.5/ 46.0  
= 8.576 mol  
Number of molecules = amount x $6.022 \times 10^{23}$  
= 8.576 x $6.022 \times 10^{23}$  
= 5.16 x$10^{23}$(to 3 sig fig)

**Example 22:** There are 980mol of pure gold in a bar measuring 10 cm by 20 cm by 50 cm. What is the density of gold in kg dm$^{-3}$

Mass = amount x Mr  
= 980 x 197  
= 193060 g  
= 193.06kg  
Volume = 10x20x50  
= 10 000cm$^3$  
= 10dm$^3$  
density = mass/volume  
= 193/10  
= 19.3 kg dm$^{-3}$

Density

Density calculations are usually used with pure liquids but to work out the mass from a measured volume. It can also be used with solids and gases.

**density = mass/Volume**

Density is usually given in g cm$^{-3}$

Care needs to be taken if different units are used.
Converting quantities between different substances using a balanced equation

\[ \text{N}_2 + 3\text{H}_2 \rightarrow 2\text{NH}_3 \]

The balancing (stoichiometric) numbers are mole ratios

\( e.g. \) 1 mol of \( \text{N}_2 \) reacts with 3 mol of \( \text{H}_2 \) to produce 2 mol of \( \text{NH}_3 \)

### Example 23: What mass of Carbon dioxide would be produced from heating 5.50 g of sodium hydrogen carbonate?

\[ 2\text{NaHCO}_3 \rightarrow \text{Na}_2\text{CO}_3 + \text{CO}_2 + \text{H}_2\text{O} \]

**Step 1:** work out amount, in mol, of sodium hydrogen carbonate

\[
\text{amount} = \frac{\text{mass}}{\text{Mr}} = \frac{5.5}{84} = 0.0655 \text{ mol}
\]

**Step 2:** use balanced equation to give amount in mol of \( \text{CO}_2 \)

2 moles \( \text{NaHCO}_3 \) : 1 moles \( \text{CO}_2 \)

So 0.0655 \( \text{HNO}_3 \) : 0.0328 mol \( \text{CO}_2 \)

**Step 3:** work out mass of \( \text{CO}_2 \)

\[
\text{Mass} = \text{amount} \times \text{Mr} = 0.0328 \times 44.0 = 1.44 \text{ g}
\]

### Example 24: 23.6 cm³ of \( \text{H}_2\text{SO}_4 \) neutralised 25.0 cm³ of 0.150 M NaOH. What is the concentration of the \( \text{H}_2\text{SO}_4 \)?

\[ \text{H}_2\text{SO}_4 + 2\text{NaOH} \rightarrow \text{Na}_2\text{SO}_4 + 2\text{H}_2\text{O} \]

**Step 1:** work out amount, in mol, of sodium hydroxide

\[
\text{amount} = \text{conc} \times \text{vol} = 0.150 \times 0.025 = 0.00375 \text{ mol}
\]

**Step 2:** use balanced equation to give moles of \( \text{H}_2\text{SO}_4 \)

2 moles \( \text{NaOH} \): 1 moles \( \text{H}_2\text{SO}_4 \)

So 0.00375 \( \text{NaOH} \) : 0.001875 mol \( \text{H}_2\text{SO}_4 \)

**Step 3:** work out concentration of \( \text{H}_2\text{SO}_4 \)

\[
\text{conc} = \frac{\text{amount}}{\text{Volume}} = \frac{0.001875}{0.0236} = 0.0794 \text{ mol dm}^{-3}
\]

### Example 25: What is the total volume of gas produced in dm³ at 333K and 100 kPa when 0.651 g of magnesium nitrate decomposes when heated?

\( \text{2Mg(NO}_3)_2(s) \rightarrow 2 \text{MgO}(s) + 4\text{NO}_2(g) + \text{O}_2(g) \)

**Step 1:** work out moles of magnesium nitrate

\[
\text{amount} = \frac{\text{mass}}{\text{Mr}} = \frac{0.651}{148.3} = 0.00439 \text{ mol}
\]

**Step 2:** use balanced equation to give moles of gas produced

2 moles \( \text{Mg(NO}_3)_2 \): 4 moles \( \text{NO}_2 \) + 1 mole \( \text{O}_2 \)

So 0.00439 \( \text{Mg(NO}_3)_2 \) : 0.01098 (0.00439 x 4/2) moles gas

**Step 3:** work out volume of gas

\[
\text{Volume} = \frac{nRT}{P} = \frac{(0.01098 \times 8.31 \times 333)}{100000} = 0.303 \text{ dm}^3
\]

### Example 26: What mass of Copper would react completely with 150 cm³ of 1.60 M nitric acid?

\[ 3\text{Cu} + 8\text{HNO}_3 \rightarrow 3\text{Cu(NO}_3)_2 + 2\text{NO} + 4\text{H}_2\text{O} \]

**Step 1:** work out amount, in mol, of nitric acid

\[
\text{amount} = \text{conc} \times \text{vol} = 1.60 \times 0.15 = 0.24 \text{ mol}
\]

**Step 2:** use balanced equation to give moles of \( \text{Cu} \)

8 moles \( \text{HNO}_3 \): 3 moles \( \text{Cu} \)

So 0.24 \( \text{HNO}_3 \) : 0.09 (0.24 x 3/8) mol \( \text{Cu} \)

**Step 3:** work out mass of \( \text{Cu} \)

\[
\text{Mass} = \text{amount} \times \text{Mr} = 0.09 \times 63.5 = 5.71 \text{ g}
\]
Example 27  What is the maximum mass of Titanium that could be produced from reacting 100 g of TiCl₄ with 80 g of sodium

\[
\text{TiCl}_4 + 4 \text{ Na} \rightarrow 4 \text{ NaCl} + \text{ Ti}
\]

Step 1: work out amount, in mol, TiCl₄

\[
\text{amount} = \frac{\text{mass}}{\text{Mr}} = \frac{100}{189.9} = 0.527 \text{ mol}
\]

Step 2: use balanced equation to work out which reactant is in excess

Using 1TiCl₄:4 Na ratio we can see that 0.527mol of TiCl₄ should react with 2.108 mol of Na. We actually have 3.48 mole of Na which is an excess of 1.372 moles. We can complete calculation using the limiting reactant of TiCl₄

Step 3: use balanced equation to work out amount in mol of Ti formed

1 mol TiCl₄: 1 mole Ti
So 0.527mol TiCl₄ produces 0.527 mole Ti

Step 4: work out mass of Ti formed

\[
\text{Mass} = \text{amount} \times \text{Mr} = 0.527 \times 47.9 = 25.24 \text{ g}
\]

Example 28: 25.0g of Fe₂O₃ was reacted and it produced 10.0g of Fe. What is the percentage yield?

\[
\text{Fe}_3\text{O}_4 + 3\text{CO} \rightarrow 2\text{Fe} + 3\text{CO}_2
\]

First calculate maximum mass of Fe that could be produced

Step 1: work out amount in mol of Iron oxide

\[
\text{amount} = \frac{\text{mass}}{\text{Mr}} = \frac{25}{159.6} = 0.1566 \text{ mol}
\]

Step 2: use balanced equation to give moles of Fe

1 moles Fe₂O₃ : 2 moles Fe
So 0.1566 Fe₂O₃ : 0.313 moles Fe

Step 3: work out mass of Fe

\[
\text{Mass} = \text{amount} \times \text{Mr} = 0.313 \times 55.8 = 17.48 \text{ g}
\]

% Yield

\[
\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100
\]

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

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

Example 29: What is the % atom economy for the following reaction where Fe is the desired product assuming the reaction goes to completion?

\[
\text{Fe}_2\text{O}_3 + 3\text{CO} \rightarrow 2\text{Fe} + 3\text{CO}_2
\]

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

= 45.8%

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

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. \(\text{CH}_2=\text{CH}_2 + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_3\)

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.