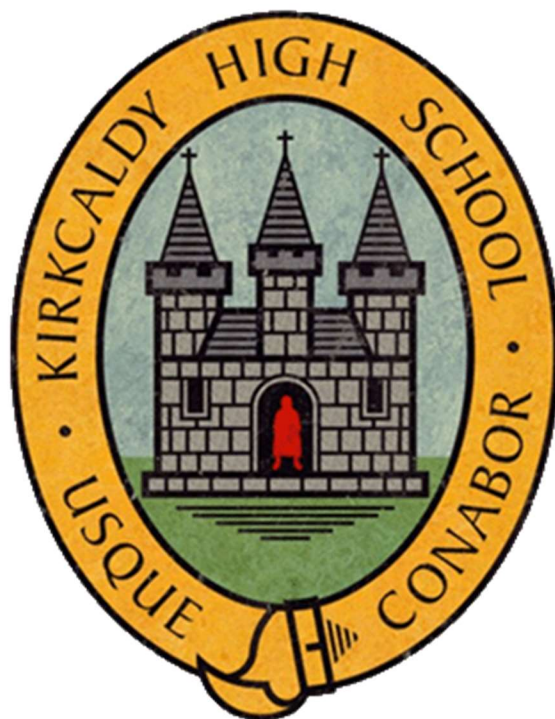# Kirkcaldy High School

Chemistry

Higher

Unit 3 – Chemistry in Society

NOTES

Course Overview

Contents

The Higher Course is split into three units. *Italic* shows the contents of this notes booklet.

Unit 1 – Chemical Changes in Structure

    (a) Periodicity

    (b) Structure and Bonding

    (c) Oxidising and Reducing Agents

Unit 2 – Nature's Chemistry

    (a) Systematic Carbon Chemistry

    (b) Alcohols

    (c) Carboxylic Acids

    (d) Esters, Fats, and Oils

    (e) Soaps, Detergents, and Emulsions

    (f) Proteins

    (g) Oxidation of Food

    (h) Fragrances

    (i) Skin Care

Unit 4 – Researching Chemistry

    (a) Common Chemical Apparatus

    (b) General Practical Techniques

    (c) Reporting Experimental Work

Assessment

- There is a **final exam** for Higher Chemistry. It is split into **two papers**:
    - Paper 1: Multiple Choice, 25, marks, 40 mins
    - Paper 2: Written Answers, 95, marks, 2 h 20 min
    - 75 marks of written answer questions
- There is an **Assignment** (essay on a Chemistry topic) to write for National 5 Chemistry.
    - The Assignment is **externally marked** by an SQA marker (NOT your teacher)
    - The Assignment contains **20 marks,** but these are scaled to 30 marks such that the assignment is worth 20 % of the total marks.
    - You have unlimited **time to research** and gather data for your Assignment.
    - You can 2 **h to write** the Assignment.

(a) Getting the Most from Reactants

When designing the practical route required to produce a marketable product, there are several key considerations.

- availability and cost of **feedstocks**
- sustainability of feedstocks
- size of yield
- formation of side products that can be recycled, used in the process or sold to increase profit

Processes in the chemical industry need to consider the environmental impact of the reactions they are undertaking. Chemical companies must seek to minimise waste by recycling where possible while avoiding either using or producing toxic chemicals.

While waste is often unavoidable, producing waste that can decompose or biodegrade naturally is preferable.

Mole ratio

A balanced chemical equation can be used to show how the quantities of reactants relate to the quantities of products in the reaction.

Consider the following reaction:

Aluminium can be obtained from aluminium ore (Al_2O_3) by a process called electrolysis. Oxygen is also produced by this reaction.

The balanced equation for this process is:

$$2Al_2O_3(aq) \rightarrow 4Al(s) + 3O_2(g)$$

The equation shows you that for every two moles of aluminium oxide oxidised, four moles of aluminium metal are obtained along with three moles of oxygen gas.

The formula mass of each reactant or product can be used to calculate the reacting masses.

Mole ratio Example – calculating mass of product formed from mass of reactant

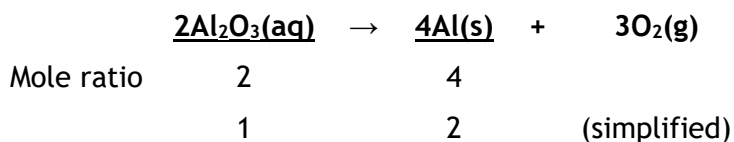Calculate the mass of aluminium formed when 51 g of aluminium oxide are electrolysed.

$$2Al_2O_3(aq) \rightarrow 4Al(s) + 3O_2(g)$$

Step 1

Underline aluminium and aluminium oxide

$$\underline{2Al_2O_3(aq)} \rightarrow \underline{4Al(s)} + 3O_2(g)$$

Step 2

Write the mole ratio underneath them

$$\underline{2Al_2O_3(aq)} \rightarrow \underline{4Al(s)} + 3O_2(g)$$

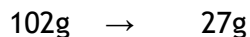|		
Mole ratio	2	4
	1	2 (simplified)

Step 3

Find the formula mass of aluminium oxide and aluminium using the formula and masses found in the data book.

$$\underline{2Al_2O_3(aq)} \rightarrow \underline{4Al(s)} + 3O_2(g)$$

Mole ratio	1	1
GFM	102	27
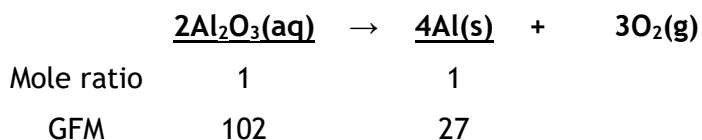
Step 4   **Al = 27g**

102g of aluminium oxide produce 27g of aluminium

$$102g \rightarrow 27g$$

To calculate the mass of aluminium formed when 51 g of aluminium oxide are electrolysed we first find what 1g would form, then find for 51g:

$$\textbf{102g} \rightarrow \textbf{27g}$$

$$1g \rightarrow \frac{27}{102}$$

$$51g \rightarrow \frac{27}{102} \times 51 = \textbf{13.5g}$$
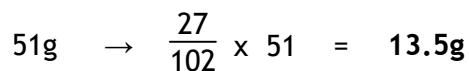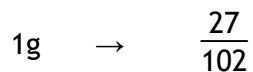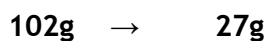
Molar volume

The molar volume is the volume occupied by one mole of any gas. The same value is obtained for all gases at the same temperature and pressure.

The value of the molar volume will be different for different temperatures and pressures and it is **measured in litres per mole** $(l\ mol^{-1})$.

As one mole of every gas will occupy the same volume at a given temperature and pressure, we can use volumes and the molar ratio to calculate volumes of reactants or products.

Consider the following reaction:

Ammonia (NH_3), which is both a useful and profitable compound, can be produced in the chemical industry from the relatively cheap reactants nitrogen and hydrogen. The balanced equation for this process is:

$$N_2(g) \quad + \quad 3H_2(g) \quad \rightarrow \quad 2NH_3(g)$$
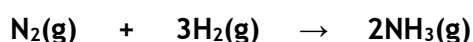
Molar volume Example (Usually found in multiple choice section)

e.g. When 400 cm^3 of nitrogen reacts with excess hydrogen, calculate the volume of ammonia that will be produced.
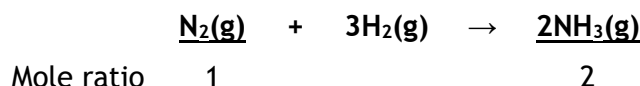
Step 1 Underline nitrogen and ammonia

$$\underline{N_2(g)} \quad + \quad 3H_2(g) \quad \rightarrow \quad \underline{2NH_3(g)}$$
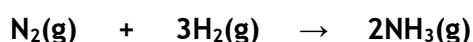
Step 2

Write the mole ratio underneath them.

Looking at the balanced equation, we can see that one mole of nitrogen reacting results in the formation of two moles of ammonia.

	$\underline{N_2(g)}$	+	$3H_2(g)$	$\rightarrow$	$\underline{2NH_3(g)}$
Mole ratio	1				2

The question does not give us information about the masses involved, but since the products and reactants are at the same temperature and pressure and are both **gases**, we know that one mole of each product and reactant will occupy the same volume
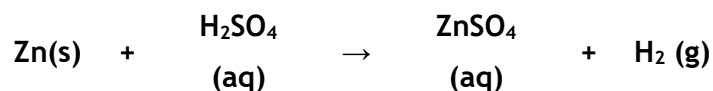
Step 3

The molar ratio of nitrogen to ammonia from the balanced equation is 1:2. This means that if 400 cm^3 of nitrogen are used then we will form double that volume of ammonia.

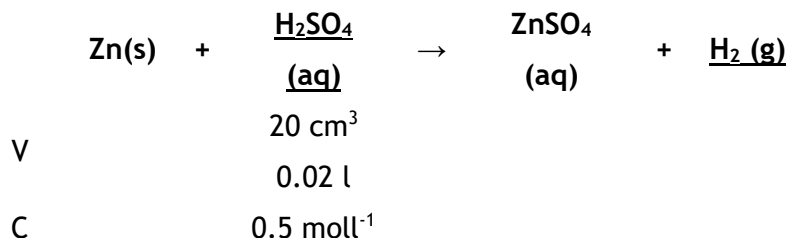|	$\underline{N_2(g)}$	+	$3H_2(g)$	$\rightarrow$	$\underline{2NH_3(g)}$
Mole ratio	1				2
Gas Volume	400 cm^3				**800 cm^3**
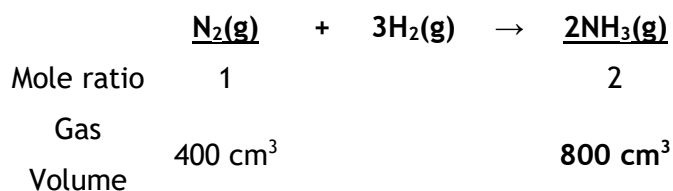
Molar volume Example - Working out the volume of product formed from a mass of reactant

e.g. What volume of hydrogen would be produced if 20.0 cm^3 H$_2$SO$_4$, concentration 0.5 mol l^{-1} reacts completely with excess zinc? (molar gas volume is 22.4 litres mol^{-1})
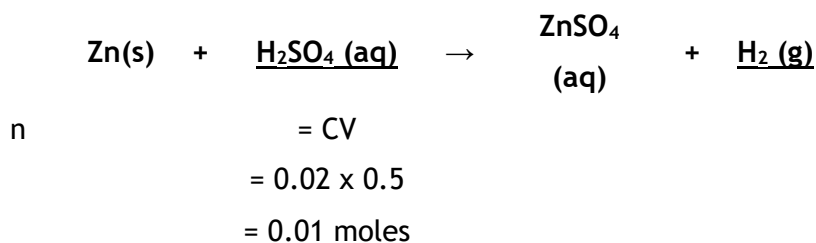
$$Zn(s) \quad + \quad \begin{matrix} H_2SO_4 \\ (aq) \end{matrix} \quad \rightarrow \quad \begin{matrix} ZnSO_4 \\ (aq) \end{matrix} \quad + \quad H_2\ (g)$$

Step 1

Underline what you are dealing with – H$_2$SO$_4$ and H$_2$ and write down what you know

$$Zn(s) \quad + \quad \begin{matrix} \underline{H_2SO_4} \\ \underline{(aq)} \end{matrix} \quad \rightarrow \quad \begin{matrix} ZnSO_4 \\ (aq) \end{matrix} \quad + \quad \underline{H_2\ (g)}$$

	20 cm^3
V	0.02 l
C	0.5 moll^{-1}

Step 2

Work out what you can: H$_2$SO$_4$ number of moles = c x v = 0.02 x 0.5 = 0.01

$$Zn(s) \quad + \quad \underline{H_2SO_4\ (aq)} \quad \rightarrow \quad \begin{matrix} ZnSO_4 \\ (aq) \end{matrix} \quad + \quad \underline{H_2\ (g)}$$

n   = CV
               = 0.02 x 0.5
               = 0.01 moles

Step 3

Write the mole ratio:

$$Zn(s) \quad + \quad \underline{H_2SO_4\ (aq)} \quad \rightarrow \quad \begin{matrix} ZnSO_4 \\ (aq) \end{matrix} \quad + \quad \underline{H_2\ (g)}$$

mole ratio   1   1

n   0.01 moles   0.01 moles

6
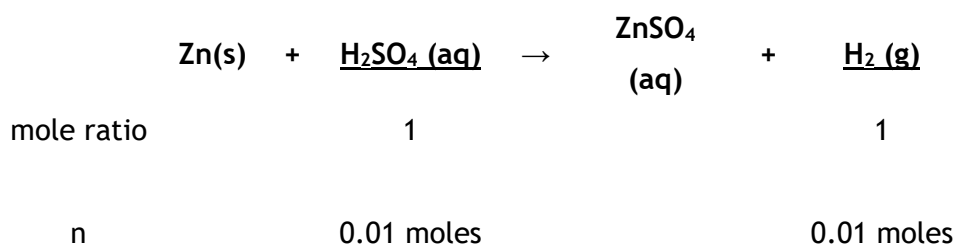
Step 4

Now you have the number of moles of H_2. Use molar volume for H_2 as it is a gas and cross multiply.

Moles Volume

$$1 \text{ mole} \quad \rightarrow \quad 24$$
$$0.01 \text{ mole} \quad \rightarrow \quad x$$

$$1x \quad = \quad \frac{24 \ x}{0.01}$$

$$x \quad = \quad \frac{0.01 \times 24}{1}$$

$$x \quad = \quad 0.24 \ l$$

Percentage yield

The percentage yield of a chemical reaction is an important consideration in industrial chemistry.

It can be calculated to compare the yield (quantity) of product actually obtained with what could have been obtained in theory, if all of the reactants were converted with no loss or waste.

Obviously **total conversion under ideal circumstances will be 100 per cent**, but in reality, that will not happen.

The formula for the percentage yield calculation as found in the data booklet is:

$$\% \text{ yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100$$

The higher the percentage yield is, the more efficient the reaction.

e.g. 5 g of methanol (CH_3OH, formula mass = 32 g) reacts with excess ethanoic acid (CH_3COOH) to produce 9.6 g of methyl ethanoate (CH_3OOCCH_3, formula mass = 74 g). Calculate the percentage yield.

Step 1
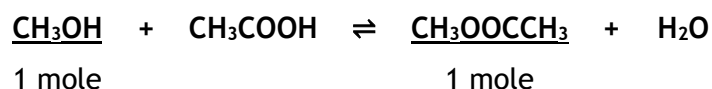
Find the actual yield which is always given in the question.

It says that **9.6 g of methyl ethanoate are produced** – this is the **actual yield.**

Step 2

Underline methanol and methyl ethanoate. Write the mole ratio below them.

The balanced equation for the reaction shows that one mole of methanol can produce one mole of methyl ethanoate.
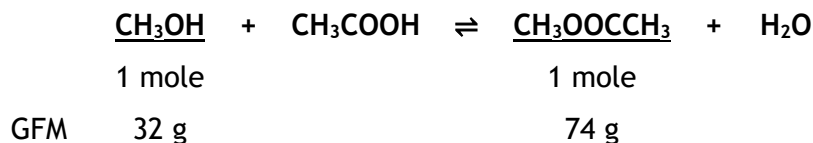
$$\underline{CH_3OH} \quad + \quad CH_3COOH \quad \rightleftharpoons \quad \underline{CH_3OOCCH_3} \quad + \quad H_2O$$
$$\text{1 mole} \qquad\qquad\qquad\qquad\qquad\quad \text{1 mole}$$

We ignore ethanoic acid as it is in excess.

Step 3

Work out the **theoretical yield** from the equation.

Underneath the mole ratio, calculate the formula mass of methanol and methyl ethanoate.

$$\underline{CH_3OH} \quad + \quad CH_3COOH \quad \rightleftharpoons \quad \underline{CH_3OOCCH_3} \quad + \quad H_2O$$

	1 mole		1 mole	
GFM	32 g		74 g	

So 32g of methanol should in theory produce 74g of methyl ethanoate, but from the question we have only used 5g of methanol.

We now work out for 1g, then 5g:

$$1g \quad \rightarrow \quad \frac{74}{32}$$

$$5g \quad \rightarrow \quad \frac{74}{32} \times 5 \quad = \textbf{11.6g}$$

Step 4

Now that we have the actual yield and theoretical yield we can put them into the equation:

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

$$\% \text{ yield} \quad = \quad \frac{9.6}{11.6} \times 100$$

$$\% \text{ yield} \quad = \quad \textbf{83 \%}$$

Atom Economy

The atom economy of a chemical reaction is a measure of the percentage of reactants that become desired products.

Inefficient, wasteful processes have low atom economies.

Efficient processes have high atom economies, and are important for sustainable development, as they use fewer natural resources and create less waste.

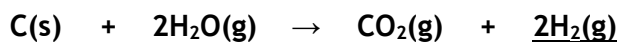The atom economy of a reaction can be calculated:

$$\textbf{\% atom economy} \quad = \quad \frac{\textbf{Mass of desired product(s)}}{\textbf{Total mass of reactants}} \times 100$$

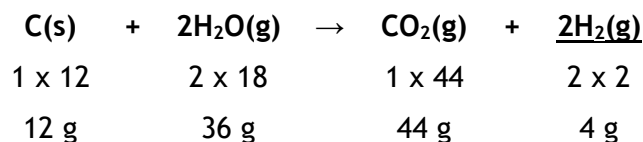**Question:** What is the atom economy for making hydrogen by reacting coal with steam?

$$C(s) \quad + \quad 2H_2O(g) \quad \rightarrow \quad CO_2(g) \quad + \quad 2H_2(g)$$
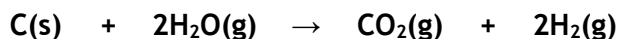
Step 1

Underline your desired product – Hydrogen

$$C(s) \quad + \quad 2H_2O(g) \quad \rightarrow \quad CO_2(g) \quad + \quad \underline{2H_2(g)}$$

Step 2

$$12 \qquad 2 \times 18 \qquad 44 \qquad 2 \times 2$$

Write the masses of all chemicals below by using m = n x gfm

$$\text{C(s)} \quad + \quad 2H_2O(g) \quad \rightarrow \quad CO_2(g) \quad + \quad \underline{2H_2(g)}$$

$$\begin{array}{cccc} 1 \times 12 & 2 \times 18 & 1 \times 44 & 2 \times 2 \\ 12\text{ g} & 36\text{ g} & 44\text{ g} & 4\text{ g} \end{array}$$

Step 3

Work out **atom economy** of Hydrogen using the equation:

$$\textbf{\% atom economy} \quad = \quad \frac{\textbf{Mass of desired product(s)}}{\textbf{Total mass of reactants}} \times 100$$

$$\% \text{ atom economy} \quad = \quad \frac{4}{12 + 36} \times 100$$

$$\% \text{ atom economy} \quad = \quad \textbf{8.3 \%}$$

This process has a **low atom economy** and is therefore an **inefficient way to make hydrogen**. It also uses coal, which is a finite (non-renewable) resource.

It is possible for chemical reactions with a high percentage yield to have a low atom economy.

This problem arises when processes have large quantities of unwanted by-products produced.

Limiting and Excess

A good way to ensure that one reactant fully reacts is to use an excess of the other reactant. This is financially efficient when one of the reactants is very cheap.

When one reactant is in excess, there will always be some left over. The other reactant becomes a limiting factor and controls how much of each product is produced.

Question: Which reactant is in excess when 0.25 g of magnesium is added to 100 cm^3 of 0.1 mol l^{-1} hydrochloric acid (HCl)?
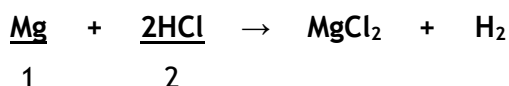
$$\text{Mg} \quad + \quad 2HCl \quad \rightarrow \quad MgCl_2 \quad + \quad H_2$$
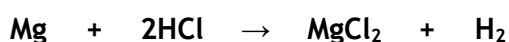
Step 1

Underline the chemicals that you have information about in the question – magnesium and hydrochloric acid.
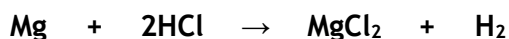
$$\underline{\text{Mg}} \quad + \quad \underline{2HCl} \quad \rightarrow \quad MgCl_2 \quad + \quad H_2$$

Step 2

Write the mole ratio below each

$$\underline{\text{Mg}} \quad + \quad \underline{2HCl} \quad \rightarrow \quad MgCl_2 \quad + \quad H_2$$
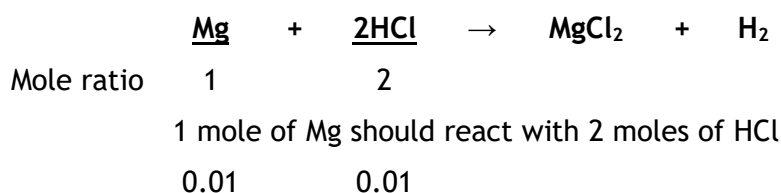$$\quad 1 \qquad\qquad 2$$

Step 3

Work out the actual number of moles used in the experiment with the information you have in the question:

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

$$n = \quad \frac{m}{GFM} \qquad\qquad CV$$

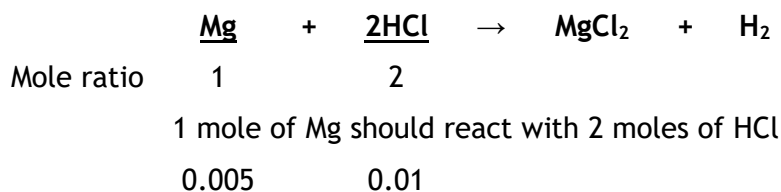$$\frac{0.25}{24.5} \qquad\qquad 0.1 \times 0.1$$

0.01 moles   0.01 moles

Step 4

Now that you have the actual number of moles used for each reactant, we go back to the mole ratio to see which one is in excess:

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

Mole ratio   1   2

1 mole of Mg should react with 2 moles of HCl

0.01   0.01

If we only have 0.01 moles of Mg it should react with double the number of HCl (0.02 moles), but we only have 0.01 moles of **HCl so it is the limiting reactant**.

Thinking of it the other way round:

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

Mole ratio   1   2

1 mole of Mg should react with 2 moles of HCl

0.005   0.01

If we only have 0.01 moles of HCl, it should react with half the number of Mg (0.005 moles), but we have 0.01 moles of **Mg so it is in excess by 0.005 moles.**

Any further calculation from this point is carried out based on the number of moles of the limiting reactant.

(b) Controlling the Rate

Collision Theory

Reactions must be controlled in industrial processes. If the rate is too low, then the process will not be economically viable (will not make money); if it is too high then there will be a risk of explosion.

For a chemical reaction to take place the reactant particles must collide successfully. For a collision to be successful particles must collide with:

1. enough energy to overcome the activation energy (E_a = The minimum kinetic energy required for a reaction to occur.)
2. The particles must collide with the correct collision geometry (angle)

When the reactant particles collide with the required activation energy (E_a) they form an activated complex. An activated complex is an unstable arrangement of atoms. These unstable intermediate breaks down to form the products of the reaction.

*e.g.* The reaction of hydrogen and bromine
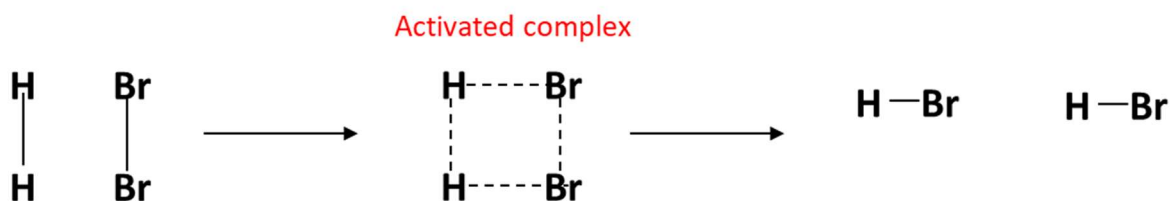
Sometimes the collisions do not result in a reaction, despite having the minimum kinetic energy. This is because the particles have not collided with the correct geometry (angle) to allow the activated complex to be formed. In the above reaction of hydrogen and bromine the particles collided side on but if they collided end on no reaction occurs as the activated complex cannot be formed if only 2 of the atoms come into contact with one another.
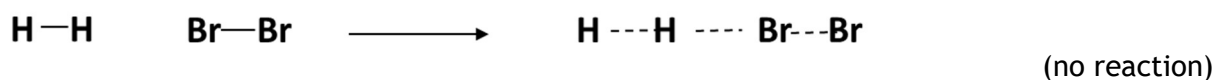
(no reaction)

Collision theory and reaction rate

Collision theory can be used to explain the effects of the following on reaction rate:
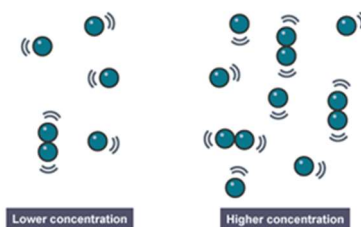
1. Particle Size: If we decrease the particle size of reactant, we increase the surface area of the reactant. More particles exposed result in greater chance of successful collisions, therefore increased rate if reaction.
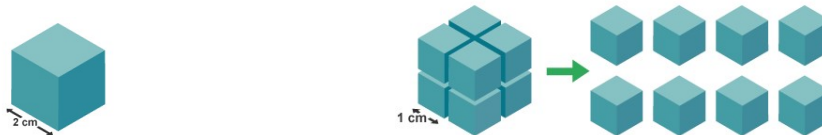

Larger particle size, smaller surface area   Smaller particle size, larger surface area

2. Concentration: If we increase the concentration of reactant, we increase the number of particles. More particles result in greater chance of successful collisions, therefore increased rate of reaction.

3. Temperature: Temperature is a measure of the average kinetic energy of all of the particles in a substance. If we increase the temperature of the reaction, we increase the speed of the particles. Particles moving at a greater speed result in more successful collisions, therefore increased rate of reaction. An increase in temperature means more particles have energy equal to or greater than the activation energy.

4. Pressure: As the pressure increases the reactant particles are pushed closer together (same number of particles in a smaller volume). Therefore, more chance of successful collision therefore increased rate of reaction.
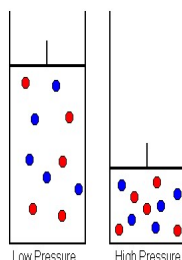

5. Catalysts: A catalyst provides the reaction with a different reaction pathway with a lower activation energy, meaning more particles have enough energy to overcome the activation energy and react. Catalysts take part in the chemical reaction but are not used up in the reaction.

Measuring the average rate of a chemical reaction

The average rate of a reaction can be measured by recording the:

1) Change in the mass of the reactants or products over a given time OR

2) Change in the volume of the reactants or products over a given time OR

[3) Change in the concentration of the reactants or products over a given time]

Measuring the change in volume of gas apparatus: (volume of gas will increase over time)

OR
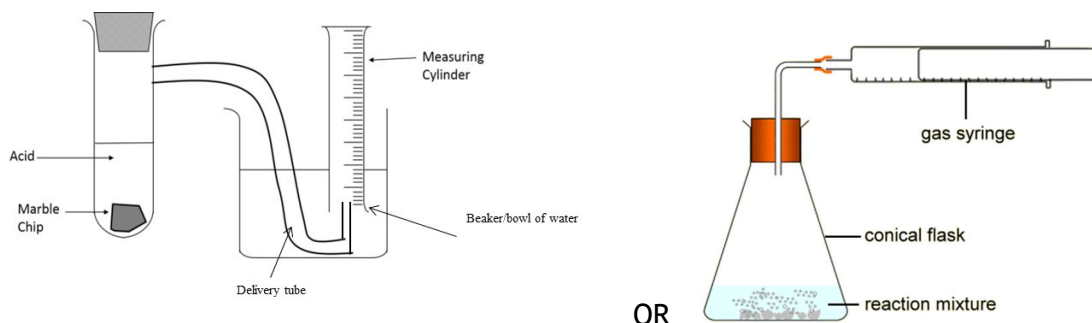
The measuring cylinder method cannot be used for gases which are soluble in water

Measuring the change in mass: (mass will decrease over time)
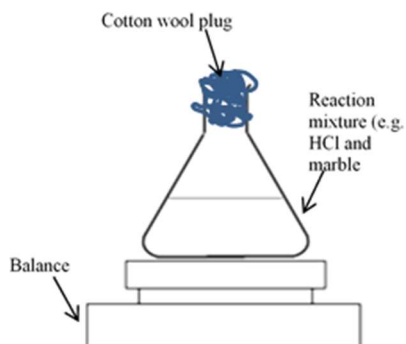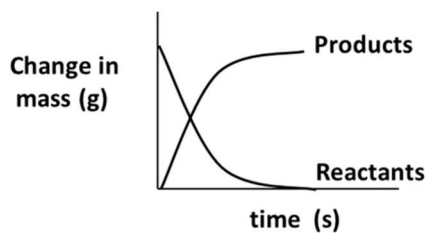

Average rate

The equation for finding the average rate of reaction is given in the front page of your data booklet.

$$\text{Average rate} = \frac{\text{change in measurable quantity}}{\text{change in time}}$$
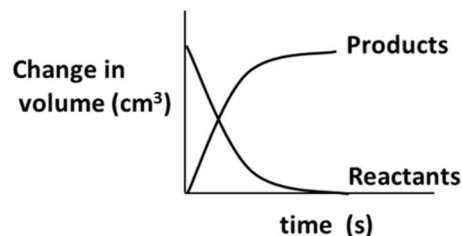
$$\text{rate} = \frac{\Delta \text{quantity}}{\Delta \text{time}}$$

(Measurable quantity = mass, volume or concentration)

Change in volume

Change in mass (g)

Products

Reactants

time (s)

Change in mass

Change in volume (cm^3)

Products

Reactants

time (s)

Average Rate = $\dfrac{\text{change in mass of product or reactant}}{\text{change in time}}$

Units g s^{-1}

Average Rate = $\dfrac{\text{change in volume of product or reactant}}{\text{change in time}}$

Units cm^3 s^{-1}

Average rates of reaction over various time intervals can show that as the reaction progresses the rate of reaction decreases (the slope/gradient of a line gives an indication of the speed). The steeper the line, the faster the reaction.

e.g.

Time (sec)	0	10	20	40	60	80
Volume of gas (cm^3)	0	17	26	71	106	135

Calculate the average rate of reaction between 20 seconds and 60 seconds.

$$\text{rate} = \frac{\Delta\text{quantity}}{\Delta\text{time}}$$

$$\text{rate} = \frac{106\text{-}26}{60\text{-}20}$$

$$\text{rate} = \frac{80}{40}$$

$$\text{rate} = \textbf{2 cm}^3\textbf{s}^{-1}$$

Relative rate

Sometimes it is difficult to measure the change in a chemical reaction (e.g. a colour change). The relative rate can be used to calculate the rate at any one point. This equation is found in the front page of your data booklet.

$$\text{relative rate} = \frac{1}{t} \qquad \text{units: s}^{-1}$$

e.g. calculate the relative rate of a reaction that took 40s to change colour.

$$\text{rate} \quad = \quad \frac{1}{t}$$

$$\text{rate} \quad = \quad \frac{1}{40}$$

$$\text{rate} \quad = \quad \textbf{0.025 s}^{-1}$$

If you know the relative rate you can work out the time

$$t \ (s) = \frac{1}{\text{rate}} \qquad \text{units: s}$$

For example, calculate the time taken for a reaction that had a rate of 0.02 s^{-1}

$$\textbf{time} \quad = \quad \frac{1}{\textbf{rate}}$$

$$\text{time} \quad = \quad \frac{1}{0.02}$$

$$\text{time} \quad = \quad \textbf{50 s}$$

These calculations can be asked by interpreting graphs. This graph shows the effect of increasing concentration with relative rate. The straight-line graph means rate is directly proportional to the concentrations of the reactants, i.e. double the concentration and you double the rate. This is true of many reactions. The faster rate is due to the increased number of successful collisions which must occur with higher concentrations of reactants.
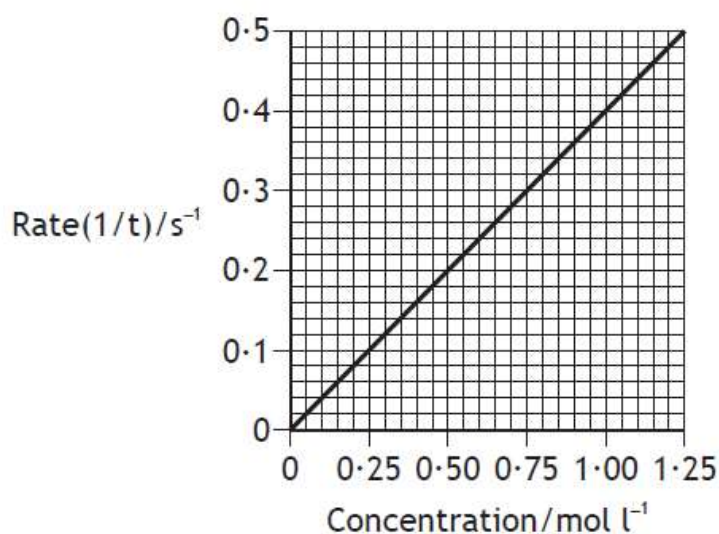
e.g. The reaction time when the concentration of the reactant was 0.5 mol l^{-1} = $\frac{1}{\text{rate}}$ = $\frac{1}{0.2}$ = **5 s**

Reaction Pathways

Potential energy diagrams can be used to show the energy pathway for a reaction.

The enthalpy change is the energy difference between the products and the reactants. It can be calculated from graphs by:
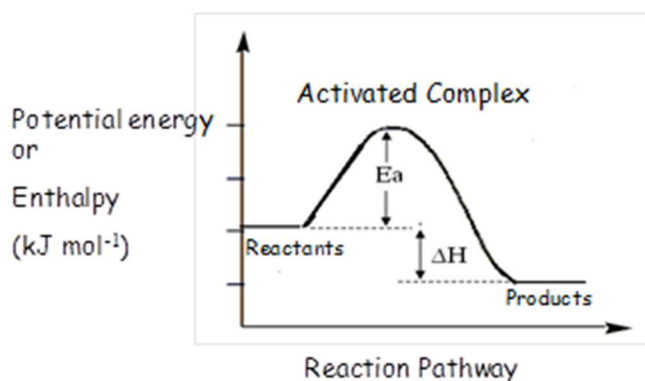
$$\Delta H = H_{products} - H_{reactants}$$

The activation energy (Ea) which is needed to start the reaction can also be calculated from graphs by:

$$Ea = H_{activated\ complex} - H_{reactants}$$

Exothermic reactions

Exothermic reaction: energy is released to the surroundings; the temperature of the surrounding usually increases. The products have less energy that the reactants. The enthalpy change, ΔH, for exothermic reactions are always negative.

Endothermic reactions

Endothermic reaction: energy is absorbed from the surroundings; the temperature of the surroundings usually decreases. The products have more energy that the reactants. The enthalpy change, ΔH, for exothermic reactions are always positive.
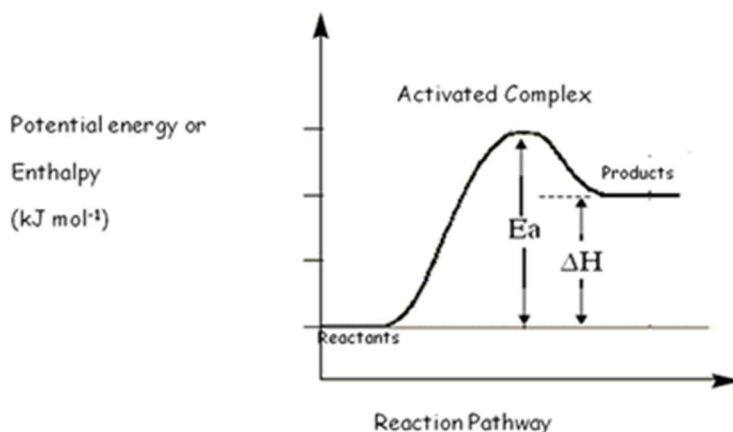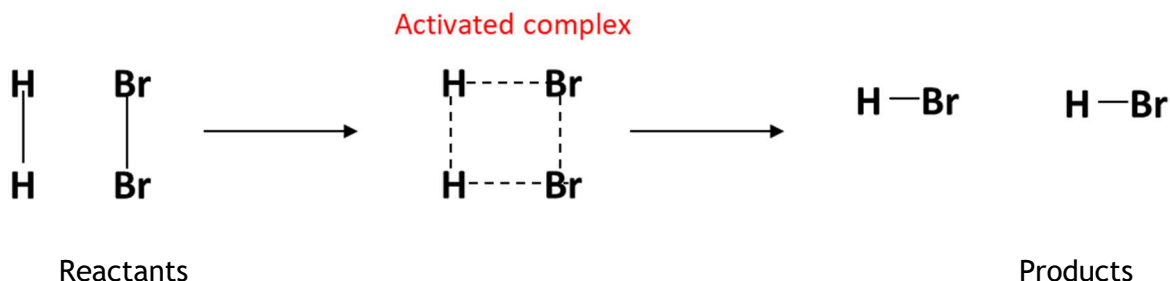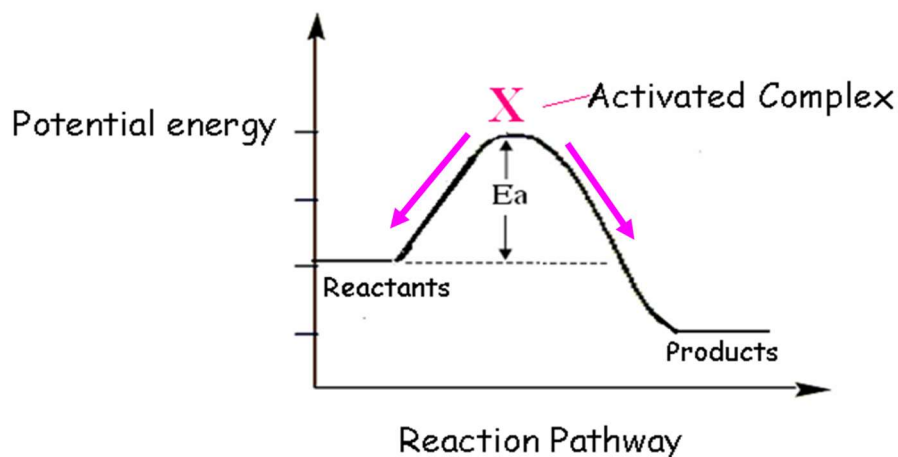

The Activated Complex

When particles collide with the required activation energy and geometry the activated complex is formed.

The activated complex is an unstable intermediate arrangement of atoms formed as old bonds are breaking and new bonds are forming.

Energy is needed to form the activated complex as bonds in the reactants may need to be broken, or charged particles brought together.

Activated complex

Reactants   Products

As the activated complex is very unstable it exists for a very short period. From the peak of the energy barrier the complex can lose energy to form either the products or the reactants again.

The higher the enthalpy change (ΔH), the more unstable the activated complex.
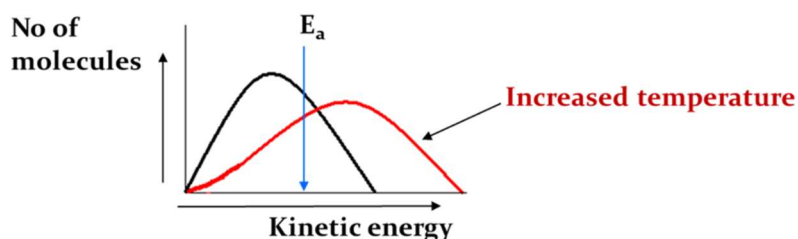
Kinetic energy distribution

Temperature is a measure of the average kinetic energy of the particles in a substance. The activation energy is the minimum kinetic energy required by colliding particles before a reaction may occur.
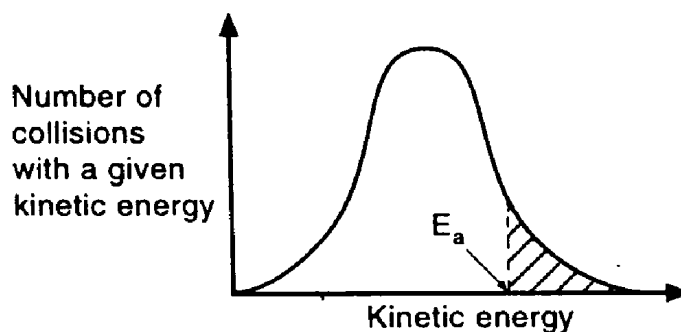
- For a pair of molecules to react the energy of the collision must be greater than the activation energy (Ea).
- The only molecules that have enough energy to react to form the activated complex and product are those in the shaded area.
- However, those particles in the shaded area may not always form products, as they may not collide with the correct collision geometry.

**Effect of temperature on energy distribution curves**

When you increase the temperature, the activation energy does not change. The number of successful collisions increases, as there are more molecules with energy greater than the activation energy and therefore the rate increases. The opposite applies for decreasing temperature.

Effect a catalyst on energy distribution curves

Catalysts speed up chemical reactions by providing an alternative reaction pathway which has a lower activation energy (activation energy decreases).
Catalysts take part in the reaction (form bonds with reactants) and are regenerated at the end of the reaction (not used up).
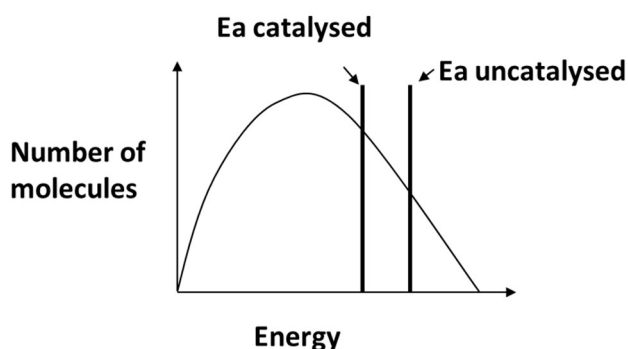
Homogeneous catalysts are in the same physical state as the reactants.
Heterogeneous catalysts are in a **different** state to the reactants.

(c) Chemical Energy

Enthalpy

- Enthalpy is a measure of the chemical energy in a substance.
- A reaction which releases heat is described as an exothermic reaction. In industry, exothermic reactions may require heat to be removed to prevent temperature rising.
- A reaction which takes in heat energy is described as endothermic. In industry, endothermic reactions may incur costs in supplying heat energy to maintain the reaction rate.
- The enthalpy change associated with a reaction can be calculated from the quantity of heat energy released.
- Combustion is a reaction when a substance burns in oxygen, releasing heat.

Enthalpy calculations

Heat energy released for a reaction can be calculated from an experiment using:

$$E_h = c \, m \, \Delta T$$

- E_h = Heat energy released (kJ)
- c = specific heat capacity of water (4.18 kJ kg^{-1} $^{\circ}$C^{-1}) = energy needed to raise the temperature of 1 kg of a substance by 1 $^{\circ}$C
- m = mass of water (kg) [we assume that 1 litre = 1 kg]
- ΔT = temperature change ($^{\circ}$C)

You may be asked to calculate the specific heat capacity for a substance other than water. If you were asked to do this, you would have to rearrange the equation $E_h = cm\Delta T$

- To find the mass of water: $m = \dfrac{E_h}{c\Delta T}$

- To find the temperature change: $\Delta T = \dfrac{E_h}{cm}$

- To find the specific heat capacity: $c = \dfrac{E}{m\Delta T}$

Enthalpy of Combustion

The enthalpy of combustion is the energy released to the surroundings when **one mole** of a substance burns completely in oxygen.

When writing balanced equations for enthalpies of combustion it is important to ensure only 1 mole of the substance being burned is included in the equation:

$$C + O_2 \rightarrow CO_2$$
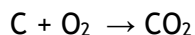
Enthalpy Calculations

There are two types of combustion calculations. In the first type the temperature difference is not mentioned, and this calculation simply requires a proportion calculation to be carried out.

e.g. When 1 g of ethanol is burned 30 kJ of energy is released. Calculate the Enthalpy of Combustion for ethanol. (remember 1 mole of substance is the same as the gfm, gfm of ethanol =46g)

$$1\ g \quad \rightarrow \quad 30\ kJ$$

$$46\ g \quad \rightarrow \quad \frac{30\ \times\ 46}{1}$$

$$1380kJ$$

This means that when 1 mole of ethanol burns it will produce 1380kJ. Since combustion is always an exothermic reaction the enthalpy of combustion is – 1380 kJmol^{-1}

Remember mass is always expressed in kg & 1cm^3 of water equals 1g

e.g. 0.16 g of methanol, CH_3OH is burned in a spirit burner. The heat from this combustion causes the temperature of 100 g of water to be raised from 20 °C to 27 °C. Calculate the enthalpy of combustion of methanol.

Step 1 E_h = c m ΔT

E_h = 4.18 x 0.1 x 7

E_h = **2.926 kJ**

Step 2   0.16g   →   **2.926kJ**

$$32g \quad \rightarrow \quad \frac{2.926\ \times\ 32}{0.16}$$

$$= \textbf{585.2 kJ}$$

So Enthalpy of Combustion, ΔH = - 585.2 kJmol^{-1}

Enthalpy of Combustion experiment

There are two problems with the experimental set up below:

- Heat is lost to the surroundings.
- Incomplete combustion occurs

(A copper can and draught shield may be used instead of a glass beaker to minimise heat loss)
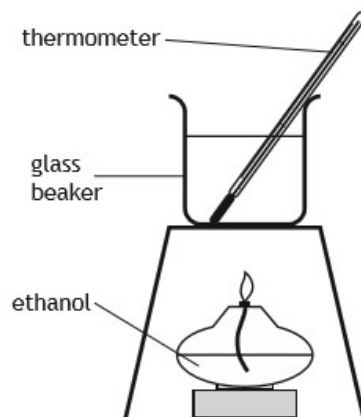
To improve the above experiment, an instrument called a bomb calorimeter can be used.

- Heat no longer lost to surroundings – water surrounds the container
- Complete combustion: calorimeter is attached to an oxygen cylinder.

Hess's Law

Hess's law states that the enthalpy change for a chemical reaction is independent of the route taken.

- The total enthalpy change for route 1 = ΔH_1
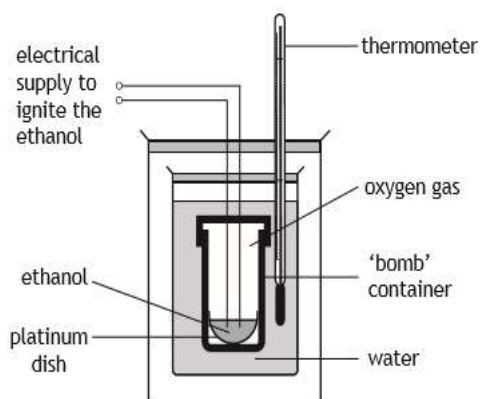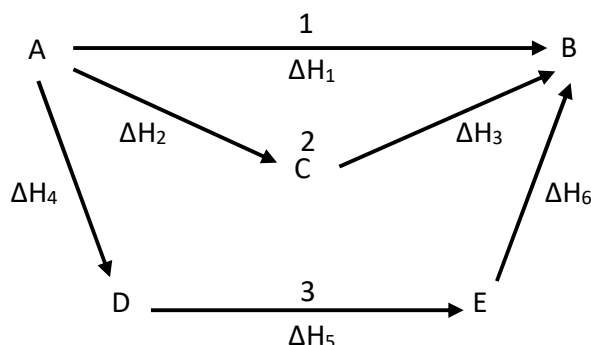- The total enthalpy change for route 2 = $\Delta H_2 + \Delta H_3$
- The total enthalpy change for route 3 = $\Delta H_4 + \Delta H_5 + \Delta H_6$
- According to Hess's Law the total enthalpy change for 1, 2 & 3 will be identical.
  - $\Delta H_1 = \Delta H_2 + \Delta H_3 = \Delta H_4 + \Delta H_5 + \Delta H_6$

Applications of Hess's Law

Hess's Law can be used to calculate enthalpy changes, which are difficult or impossible to determine, by experiment.

Hess's Law Calculations

The enthalpy of formation is the quantity of heat energy taken in or given out when 1 mole of a substance is formed from its elements in their normal state.
The information you need for a calculation will either be given in the question or can be found in the data booklet p10.
Step 1: Write out the balanced "target equation"
Step 2: Write out the balanced equations for the enthalpy of combustion of C(s), H_2(g) and what you are trying to find, and the values from the data book p10 if not given.
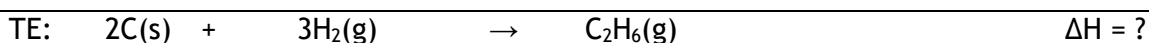**Step 3**: compare and rearrange the known equations to get the "target equation"
Step 4: cancel out and add equations and ΔH values to get the "target"

e.g. Calculate the enthalpy of formation of ethane given that the enthalpies of combustion of carbon, hydrogen and ethane are -394 kJmol^{-1}, -286 kJmol^{-1} and -1560 kJmol^{-1} respectively.
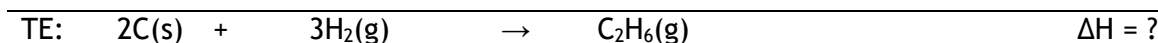
1) Write a balanced equation for the equation that you are required to calculate the enthalpy change for. This is called the Target Equation.

$$\text{TE:} \quad 2C(s) \; + \; 3H_2(g) \quad \rightarrow \quad C_2H_6(g) \qquad \Delta H = ?$$

2) Construct balanced equations for each of the substances in your target equation, using the information given in the question.

(1)	$C(s)$	+	$O_2(g)$	$\rightarrow$	$CO_2(g)$			$\Delta H = -394$
(2)	$H_2(g)$	+	$\tfrac{1}{2}O_2(g)$	$\rightarrow$	$H_2O(l)$			$\Delta H = -286$
(3)	$C_2H_6(g)$	+	$3\tfrac{1}{2}O_2(g)$	$\rightarrow$	$2CO_2(g)$	+	$3H_2O(l)$	$\Delta H = -1560$

TE:	$2C(s)$	+	$3H_2(g)$	$\rightarrow$	$C_2H_6(g)$		$\Delta H = ?$

3) These equations can now be rearranged to give the target equation. Note that whatever change you make to the equation you must also make to the enthalpy value!

(1)	$2C(s)$	+	$2O_2(g)$	$\rightarrow$	$2CO_2(g)$			$\Delta H = -394 \times 2$
(2)	$3H_2(g)$	+	$1\tfrac{1}{2}O_2(g)$	$\rightarrow$	$3H_2O(l)$			$\Delta H = -286 \times 3$
(3)	$2CO_2(g)$	+	$3H_2O(l)$	$\rightarrow$	$C_2H_6(g)$	+	$3\tfrac{1}{2}O_2(g)$	$\Delta H = +1560$
TE:	$2C(s)$	+	$3H_2(g)$	$\rightarrow$	$C_2H_6(g)$			$\Delta H = ?$

4) Cancel anything that is on both sides of the equation

(1)	$2C(s)$	+	~~$2O_2(g)$~~	$\rightarrow$	~~$2CO_2(g)$~~			$\Delta H = -394 \times 2$
(2)	$3H_2(g)$	+	~~$1\tfrac{1}{2}O_2(g)$~~	$\rightarrow$	~~$3H_2O(l)$~~			$\Delta H = -286 \times 3$
(3)	~~$2CO_2(g)$~~	+	~~$3H_2O(l)$~~	$\rightarrow$	$C_2H_6(g)$	+	~~$3\tfrac{1}{2}O_2(g)$~~	$\Delta H = +1560$
TE:	$2C(s)$	+	$3H_2(g)$	$\rightarrow$	$C_2H_6(g)$			$\Delta H = 86$ kJmol^{-1}

Once everything that appears on both the reactant side and the product side have been cancelled you should be left with your target equation!

e.g. Use the enthalpies of combustion in your data booklet to find the enthalpy change for the reaction between ethyne and hydrogen to produce ethane.
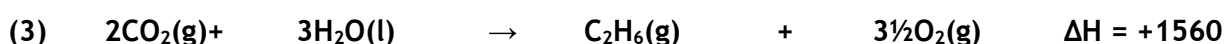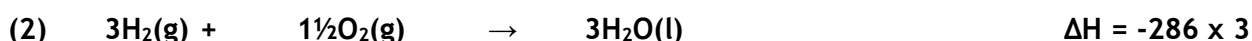
1) Write a balanced equation for the equation that you are required to calculate the enthalpy change for. This is called the Target Equation.
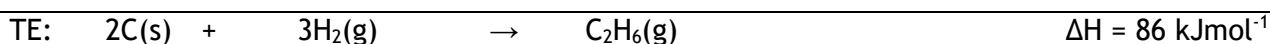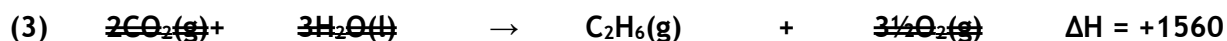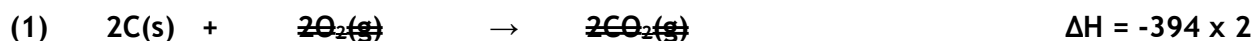
$$\text{TE:} \quad C_2H_2 + 2H_2 \rightarrow C_2H_6 \qquad \Delta H = ?$$

2) Construct balanced equations for each of the substances in your target equation, using the information given in the question.

(1)	C_2H_2	+	$2\tfrac{1}{2}O_2$	→	$2CO_2$ +	H_2O	$\Delta H = -1300$
(2)	H_2	+	$\tfrac{1}{2}O_2$	→	H_2O		$\Delta H = -286$
(3)	C_2H_6	+	$3\tfrac{1}{2}O_2$	→	$2CO_2$ +	$3H_2O$	$\Delta H = -1560$
TE:	C_2H_2	+	$2H_2$	→	C_2H_6		$\Delta H = ?$

3) These equations can now be rearranged to give the target equation. Note that whatever change you make to the equation you must also make to the enthalpy value!
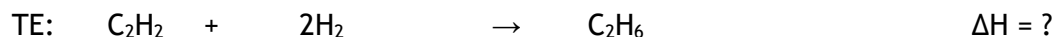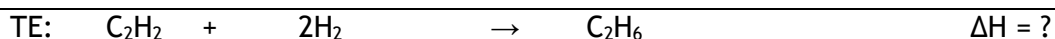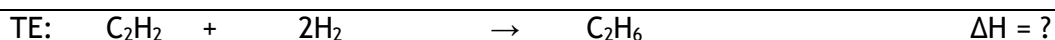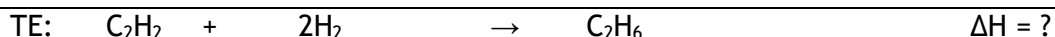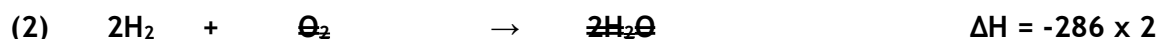
(1)	C_2H_2	+	$2\tfrac{1}{2}O_2$	→	$2CO_2$ +	H_2O	$\Delta H = -1300$
(2)	$2H_2$	+	O_2	→	$2H_2O$		$\Delta H = -286 \times 2$
(3)	$2CO_2$	+	$3H_2O$	→	C_2H_6 +	$3\tfrac{1}{2}O_2$	$\Delta H = -1560$
TE:	C_2H_2	+	$2H_2$	→	C_2H_6		$\Delta H = ?$

4) Cancel anything that is on both sides of the equation

|							
(1)	C_2H_2	+	~~$2\tfrac{1}{2}O_2$~~	→	~~$2CO_2$~~ +	~~H_2O~~	$\Delta H = -1300$
(2)	$2H_2$	+	~~O_2~~	→	~~$2H_2O$~~		$\Delta H = -286 \times 2$
(3)	~~$2CO_2$~~	+	~~$3H_2O$~~	→	C_2H_6 +	~~$3\tfrac{1}{2}O_2$~~	$\Delta H = -1560$
TE:	C_2H_2	+	$2H_2$	→	C_2H_6		$\Delta H = ?$

Once everything that appears on both the reactant side and the product side have been cancelled you should be left with your target equation!

Bond Enthalpy

Molar bond enthalpy

The molar bond enthalpy is the energy required to break one mole of bonds in a diatomic molecule. These values are given on p10 of the data booklet.

e.g. The bond enthalpy of chlorine:

$$Cl_2 \text{ (g)} \rightarrow 2Cl \text{ (g)} \qquad \Delta H= 243 \text{ kJ mol}^{-1}$$
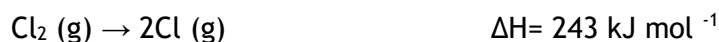
This is how much energy it takes to break the bonds of chlorine. Bond breaking is therefore endothermic. Therefore, bond making is exothermic:

$$2Cl(g) \rightarrow Cl_2(g) \qquad \Delta H= -243 \text{ kJ mol}^{-1}$$

Mean molar bond enthalpy

A mean molar bond enthalpy is the average energy required to break one mole of bonds in a compound.

For molecules with more than two atoms, such as methane, it is only possible to calculate the mean bond enthalpy since the situation is much more complex with the C–H bonds breaking off one after the other to form a different fragment of the original molecule.

The removal of the first hydrogen atom from CH_4 does not require the same energy as the removal of the second hydrogen from the CH_3 fragment and so on. The value obtained is the average or mean bond enthalpy for C–H.

e.g.

$$CH_4(g) \rightarrow \quad C(g) \quad + \quad 4H(g) \qquad \Delta H = 4 \times C\text{-}H = 1656 \text{ kJ mol}$$
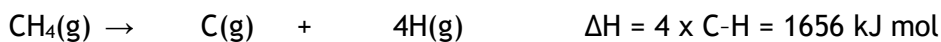
Therefore the mean bond enthalpy of C–H $= \dfrac{1656}{4}$ = 414 kJ mol^{-1}

Calculating enthalpy change for a gas phase reaction

Enthalpy change for a gas phase reaction can be calculated using:

$$\Delta H = \Sigma \Delta H_{\text{bonds broken}} + \Sigma \Delta H_{\text{bonds made}}$$

Remember: bond breaking is endothermic (*positive*), bond making is exothermic (*negative*)

(always use p10 of the data booklet for these questions, unless values given in the question).

e.g. Calculate the enthalpy change, using bond enthalpies for this reaction:

$$Cl_2 (g) + H_2 (g) \rightarrow 2HCl (g)$$
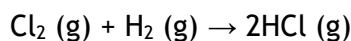
Step 1: *Work out the enthalpy of bond breaking*

In this example   **1 mole of Cl-Cl bonds break = 243 kJmol^{-1}**

1 mole of H-H bonds break = 436 kJmol^{-1}

Total = 243 + 436 = +679 kJmol^{-1}

Step 2: *Work out the enthalpy of bond making*

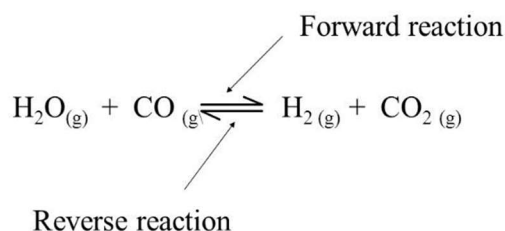In this example 2 moles of H-Cl bonds are made = 2 x -432 = **-864 kJmol^{-1}**

Step 3:

$$\Delta H \quad = \quad \Sigma \Delta H_{\text{bonds broken}} + \Sigma \Delta H_{\text{bonds made}}$$

$$\Delta H \quad = \qquad +679 + (-864)$$

$$\Delta H \quad = \qquad \textbf{-185 kJmol}^{-1}$$

(d) Equilibria

To maximise profits, chemists employ strategies to move the position of the equilibrium to favour the products (the forward reaction).

$$H_2O_{(g)} + CO_{(g)} \rightleftharpoons H_{2\,(g)} + CO_{2\,(g)}$$

Forward reaction

Reverse reaction

If the equilibrium position lies to the RIGHT more product is formed. If the equilibrium position lies to the LEFT more reactant is present.

At equilibrium:

At the start of a reaction there will be 100% reactants. However, as the reaction proceeds the reactants will be used up and the products will be formed. Eventually the reaction will reach equilibrium. At this stage the concentration of both the reactants and products will remain constant (NOT EQUAL). The reaction has reached equilibrium, NOT stopped!
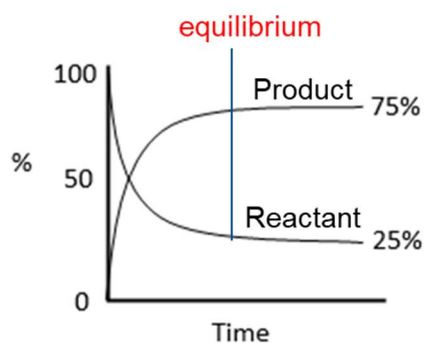
The rate of the forward reaction EQUALS the rate of the reverse reaction.
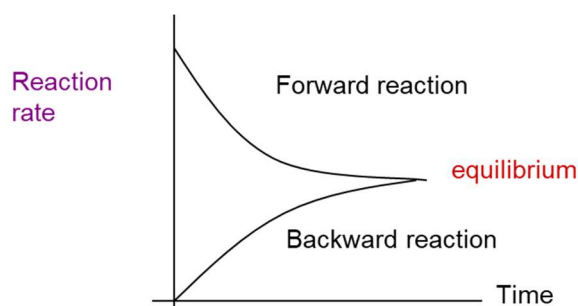
Le Chateliers's Principle

Le Chateliers's Principle States that: If a system at equilibrium is subjected to any change, the system readjusts itself to counteract the applied change.

Change	Effect on equilibrium position
Add more reactant.	Moves to the right. (Makes more product)
Add more product.	Moves to the left. (Makes more reactant)
Remove product.	Moves to the right. (Makes more product). Same effect as adding more reactant.
Remove reactant.	Moves to the left. (Makes more reactant). Same effect as adding more product.
Increase temperature.	Moves in the endothermic direction i.e. the direction where ΔH is +ve.
Decrease temperature.	Moves in the exothermic direction i.e. the direction where ΔH is –ve.
Increase pressure.	Moves to the side with the least number of moles of gas.
Decrease pressure.	Moves to the side with the most moles of gas.
Add a catalyst	No effect on equilibrium position. It just reaches this equilibrium quicker.

(e) Chemical Analysis

(i) Chromatography

Chromatography is a technique used to separate components present within a mixture. Chromatography can be used to follow the course of a chemical reaction or to establish the products of a chemical reaction.

Paper Chromatography

During paper chromatography a small sample of the mixture being tested is spotted onto the base line (a straight line usually drawn in pencil above the level of the solvent) on the filter paper. The filter paper is then placed in a solvent.

By capillary action the solvent moves up the paper. This is when different components of the mixture are separated.

Components can move quickly or slowly up the paper depending on the solvent used.

There are two stages in paper chromatography; the Mobile Phase and the Stationary Phase.

The solvent is the mobile phase in paper chromatography and the wet paper is the stationary phase.
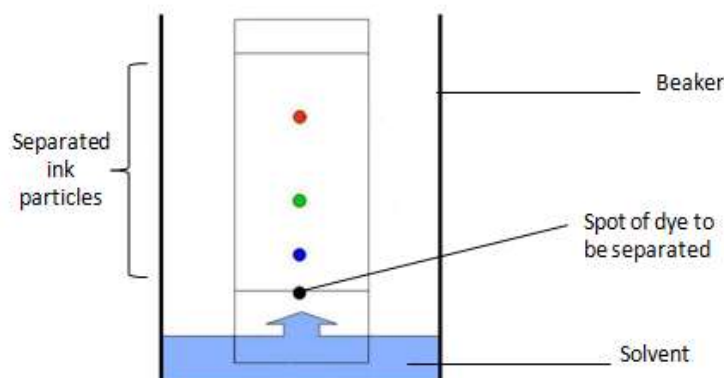
Separation

Separation occurs due to polarity and size of molecules:
* Larger molecules do not move as quickly
* In a polar solvent, polar molecules will move more quickly as the polar molecule is more strongly attracted to the mobile phase.

The Retention Factor (Rf) Values

The Rf factor can be used to compare the different components found in a sample. The Rf values of a mixture being tested can be compared with known samples.
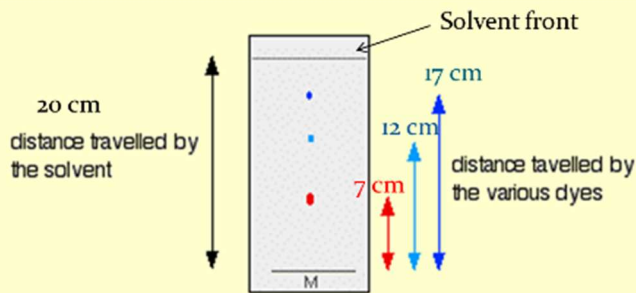
$$R_f = \frac{\text{distance travelled by component}}{\text{distance travelled by solvent}}$$

R_f for first spot: 7/20=0.35

R_f for last spot: 17/20=0.85

Note: if two substances on chromatography paper have the same Rf value it is likely that they are the same compound. If they do not have the same Rf value then they are definitely different compounds.

Gas Liquid Chromatography

During gas liquid chromatography, heat vaporises the sample and is carried by gas through hot column. The rate of travel through column depends on affinity for inert gas. The sample is the identified by 'retention time'.

- Stationary: High boiling point liquid
- Mobile phase: Inert gas (unreactive gas) e.g. Helium or nitrogen

The retention time is the time taken between injection of a sample and the time of elution of the component.
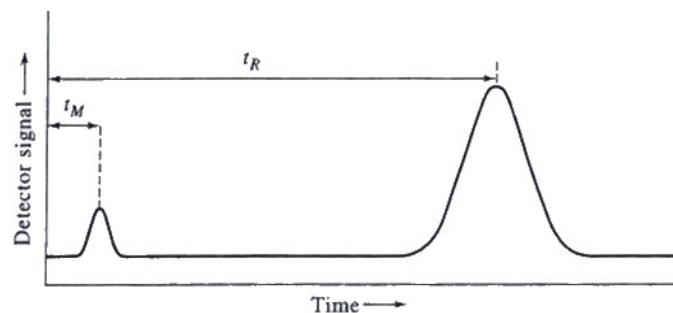
The peak area indicates concentration of substance. If the peak is off the scale the sample was too concentrated and needs diluting.
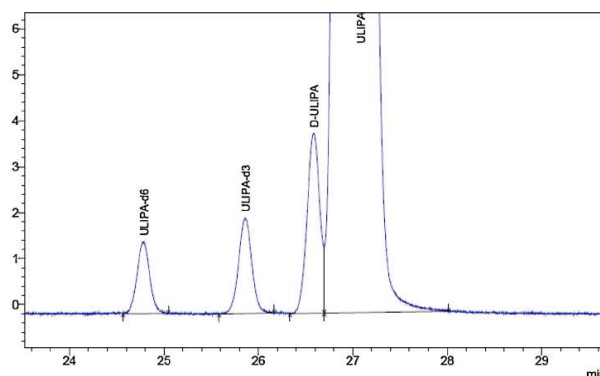
Volumetric Analysis

Redox Titrations

Titration is used to determine, accurately, the volumes of solution required to reach the end-point of a chemical reaction. An indicator is normally used to show then an end-point is reached.

For many reactions an indicator must be used however, for some redox reactions the end-point can be recognised from a colour change in one of the reactants. When potassium permanganate solution (purple) reacts with iron (II) sulphate solution, no indicator is required, and purple permanganate is self-indicating turns colourless when reduced.

Titre volumes within 0.2 cm^3 are considered concordant and are used when calculating an average. The average titre is never used as it is not accurate.
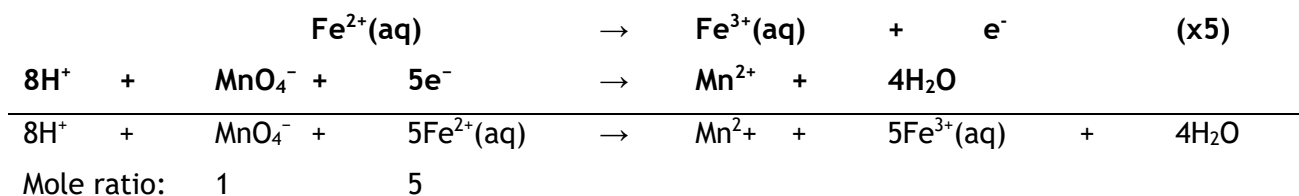
Burettes and pipettes are used in titrations to accurately measure solutions. A solution of an accurately known concentration is known as a standard solution.

Titration calculation

e.g.

20 cm^3 of iron(II)sulphate were titrated with 0.01mol-1 potassium permanganate solution until a permanent pink colour was observed. If the volume of potassium permanganate used was 25.6 cm^3, what is the concentration of the iron(II)sulphate solution?
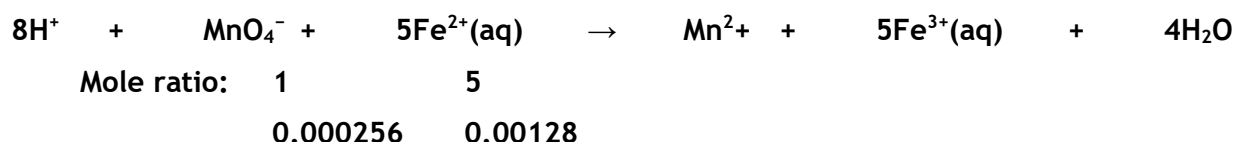
Step 1: write the ion-electron equations and combine to give the redox equation.

$$Fe^{2+}(aq) \rightarrow Fe^{3+}(aq) + e^- \quad (x5)$$

$$8H^+ + MnO_4^- + 5e^- \rightarrow Mn^{2+} + 4H_2O$$

$$8H^+ + MnO_4^- + 5Fe^{2+}(aq) \rightarrow Mn^{2+} + 5Fe^{3+}(aq) + 4H_2O$$

Mole ratio: 1   5

Step 2: calculate the number of moles of the 'known' substance (MnO_4^-)

$$n = C V$$
$$n = 0.01 \times 0.0256$$
$$n = 0.000256 \text{ moles}$$

using the mole ratio:

$$8H^+ + MnO_4^- + 5Fe^{2+}(aq) \rightarrow Mn^{2+} + 5Fe^{3+}(aq) + 4H_2O$$

Mole ratio: 1   5

0.000256   0.00128

Step 3: calculate the concentration of the iron(II)sulphate solution

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

$$C = \frac{0.00128}{0.02}$$

$$C = 0.064 \text{ mol l}^{-1}$$

Glossary

Word	Meaning
Activation energy	The minimum amount of energy needed for a reaction to begin.
Bond Dissociation Enthalpy	Energy required to break one mole of bonds to form two separate atoms, all species being in the gaseous state.
Catalyst	A chemical which speeds up a chemical reaction without being used up itself and which can be removed chemically unchanged at the end of the reaction.
Chemical reaction	An interaction between substances (chemicals) in which their atoms re-arrange to form new substances.
Concentration	The amount of particles in a given volume.
Enthalpy of Combustion	Enthalpy change when one mole of substance burns completely in oxygen.
Hess's law	The enthalpy change for a chemical reaction is independent of the route taken, providing the starting point and finishing point is the same for both routes.
Molar Volume	The volume, in litres, occupied by one mole of gas under standard conditions of temperature and pressure.
Products	The substances (chemicals) at the end of a chemical reaction.
Rate of reaction	How quickly a reactant is used up OR how quickly a product is created.
Reactants	The substances (chemicals) at the start of a chemical reaction.
Surface area	Total area of a substance which is exposed to the surroundings.