

OCR: Chemistry – Unit 2 – Chains, Energy and Resources

Note: For all Mechanisms and Reactions – There is an attached sheet at the end showing all the needed reactions in more detail.

THERE IS ALSO A LIST OF ALL EQUATIONS AND REACTION NEEDED FOR THIS SYLLABUS ATTACHED IN A SEPARATE FILE .

(a) Interpret and use the terms:

(i) Empirical formula as the **simplest whole number ratio of atoms of each element present in a compound.**

(ii) molecular formula as the **actual number of atoms of each element in a molecule,**

(iii) general formula as the simplest algebraic formula of a member of a homologous series

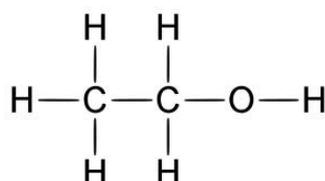
Alkane	C_nH_{2n+2}
Alkene	C_nH_{2n}
Alcohol	$C_nH_{2n+1}OH$
Cycloalkane	C_nH_{2n}
Cycloalkene	C_nH_{2n-2}
Haloalkane	$C_nH_{2n+1}X$

(iv) structural formula as **the minimal detail that shows the arrangement of atoms in a molecule**

E.g. Butane:

$CH_3CH_2CH_2CH_3$ or $CH_3(CH_2)_2CH_3$,

(v) displayed formula as **the relative positioning of atoms and the bonds between them, ie for ethanol:**



(vi) **skeletal formula as the simplified organic formula, shown by removing hydrogen atoms from alkyl chains, leaving just a carbon skeleton and associated functional group**

ie for butan-2-ol:



(b) **interpret, and use, the terms:**

(i) **homologous series as a series of organic compounds having the same functional group but with each successive member differing by CH₂,**

(ii) **functional group as a group of atoms responsible for the characteristic reactions of a compound;**

(c) use the general formula of a homologous series to predict the formula of any member of the series;

E.g – Alkane = C_nH_{2n+2}

If C = 9, H = (9x2) + 2

Therefore = C₉H₂₀ = Nonane

(d) **state the names of the first ten members of the alkanes homologous series;**

No of Carbons	Alkyl Group
1	Methyl
2	Ethyl
3	Propyl
4	Butyl
5	Pentyl
6	Hexyl
7	Heptyl
8	Octyl
9	Nonyl
10	Decyl

(f) describe and explain the terms:

(i) structural isomers as **compounds with the same molecular formula but different structural formulae,**

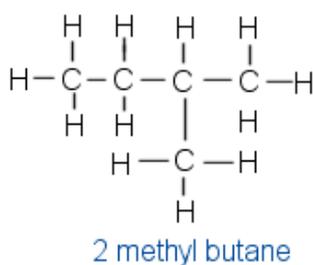
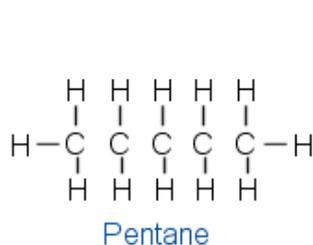
(ii) stereoisomers as **compounds with the same structural formula but with a different arrangement of atoms in space,**

(iii) E/Z isomerism as an example of stereoisomerism, in terms of **restricted rotation about a double bond and the requirement for two different groups to be attached to each carbon atom of the C=C group,**

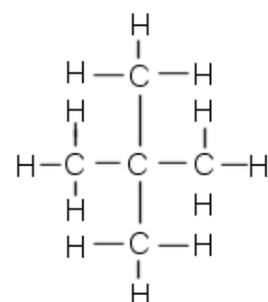
(iv) cis-trans isomerism as a special case of **EIZ isomerism in which two of the substituent groups are the same;**

(g) determine the possible structural formulae and/or stereoisomers of an organic molecule, given its molecular formula;

E.g – Pentane – C_5H_{12}



- methyl group hangs off 2nd C atom
- longest chain is 4 C's long = butane



- 2 methyl groups both hang off 2nd C atom
- longest unbroken chain is 3 C's = propane

(h) describe the different types of covalent bond fission:

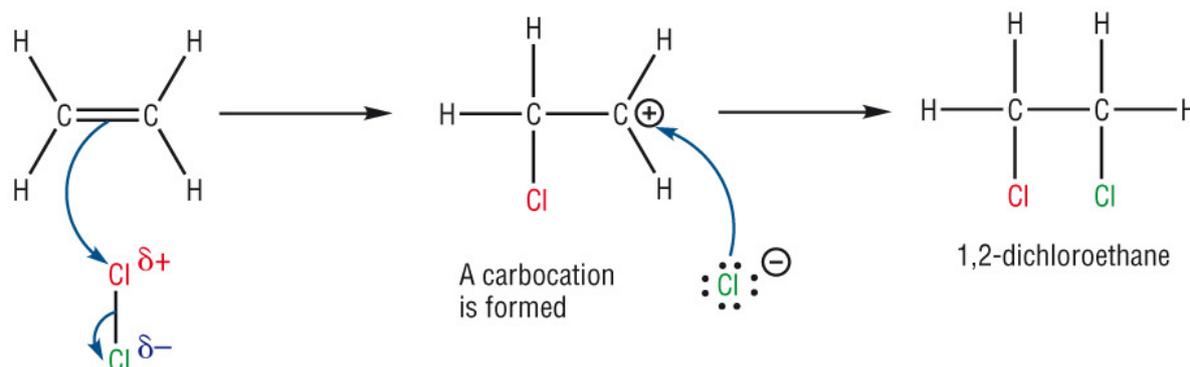
(i) homolytic fission forming two radicals,
Breaking of a covalent bond, where one electron goes to each atom

(ii) heterolytic fission forming a cation and an anion;
Breaking of a covalent bond, where both electrons go to one atom.

(i) describe a 'curly arrow' as **the movement of an electron pair, showing either breaking or formation of a covalent bond**;

(j) outline reaction mechanisms, using diagrams, to show clearly the movement of an electron pair with 'curly arrows';

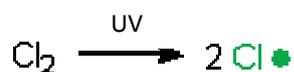
Electrophilic Addition



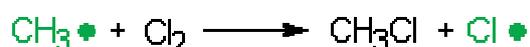
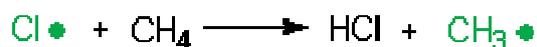
When Cl_2 approaches, the $\text{Cl}-\text{Cl}$ bond becomes polar. A pair of electrons flows from the double bond to the slightly positive $\text{Cl}^{\delta+}$ and a bond formed.

Radical Substitution

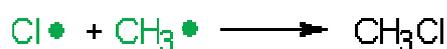
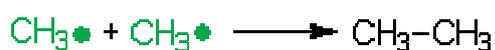
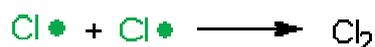
1. Initiation reaction

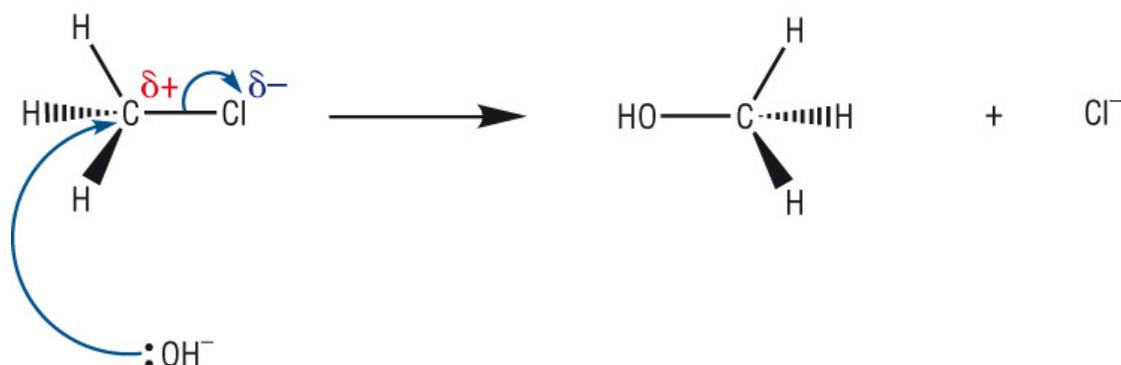


2. Chain propagation



3. Chain termination reactions



Nucleophilic Substitution

The nucleophile attacks the back of the carbon atom donating an electron pair. This causes a new bond to form and the carbon halogen bond to break.

(k) carry out calculations to determine the percentage yield of a reaction;

$$\frac{\text{Actual amount produced}}{\text{Theoretical Amount produced}} \times 100 = \text{Percentage Yield}$$

(l) explain the atom economy of a reaction as:

$$\frac{\text{Molecular Mass of desired products}}{\text{Molecular mass of all products}} \times 100$$

(m) explain that **addition reactions have an atom economy of 100%, whereas substitution reactions are less efficient;**

(a) explain that a hydrocarbon is a **compound of hydrogen and carbon only;**

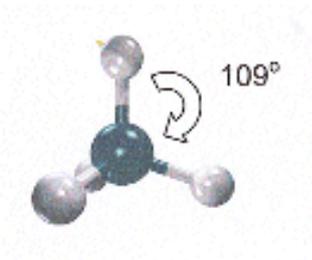
(b) explain the use of **crude oil as a source of hydrocarbons, separated as fractions with different boiling points by fractional distillation, which can be used as fuels or for processing into petrochemicals**

(c) state that **alkanes and cycloalkanes are saturated hydrocarbons;**

(d) state and explain the tetrahedral shape around each carbon atom in alkanes

The pairs of electrons in covalent bonds repel each other and so arrange themselves around the carbon atom as far apart as possible.

The C-H bonds in methane are directed so that they form a tetrahedron shape, with bond angles of 109°



(e) explain, in terms of van der Waals' forces, the variations in the boiling points of alkanes with different carbon-chain length and branching;

As the chain length increases, boiling point increases

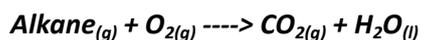
- **More intermolecular (van der Waals' forces)**
- **More points of contact**
- **More energy needed to break bonds.**

As branching increases, boiling point decreases.

- **Fewer points of contact**
- **Fewer van der Waals' forces**
- **Less energy needed to break bonds.**

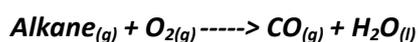
(f) describe the combustion of alkanes, leading to their use as fuels in industry, in the home and in transport;

- **Short chained alkanes are valuable as clean fuels.**
- **They burn in plentiful supply of oxygen**
- **Methane is a main constituent, used for domestic heating and cooking.**



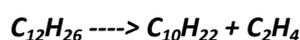
(g) explain, using equations, the incomplete combustion of alkanes in a limited supply of oxygen and outline the potential dangers arising from production of CO in the home and from car use;

- **Combustion in engines can have a limited supply of O₂**
- **Carbon Monoxide is produced (clear, colourless gas)**
- **Prevents haemoglobin binding to oxygen, starving tissues of oxygen**
- **CO can be formed from faulty heating systems, blocked chimneys, or inadequate ventilation.**



(h) describe the use of catalytic cracking to obtain more useful alkanes and alkenes;

- **Long chained hydrocarbons ----> Shorter chain alkanes + Shorter chain alkenes**
- **Shorter chain alkanes used as fuels**
- **Shorter chained alkenes used as polymer production**
- **Zeolite Catalyst + 450°C**



(i) explain that the petroleum industry processes straight-chain hydrocarbons into branched alkanes and cyclic hydrocarbons to promote efficient combustion;

- **Isomerisation used to produce branched or cyclic alkanes.**
- **Branched and cyclic alkanes burn more efficiently**

(j) contrast the value of fossil fuels for providing energy and raw materials with:

(i) the problem of an over-reliance on non-renewable fossil fuel reserves.

Currently, 90% of our fuels come from the non renewable crude oil. Our over-reliance of crude oil is a problem as we currently have no sustainable alternatives, and the Earth's deposits of crude oil are depleting rapidly.

(ii) the importance of developing renewable plant based fuels, ie alcohols and biodiesel (see also 2.4.2),

Bio fuels are fuels derived from recently living material such as plants, or from animal waste. The idea of these types of fuels is that they will be renewable, fast and easy to be produced and can be relatively cheap.

We need these types of fuels to be available for the future as our current sources of energy are depleting rapidly.

Some sources are:

- **Sugar Cane**
- **Ethanol – Made by fermentation of sugar and other carbohydrates.**
 - **Combusts efficiently in a plentiful supply of oxygen**
 - **Can be mixed with petroleum leading to further deficiency**
 - **Used as Bio ethanol in the UK, 105,000 tonnes produced per year.**
- **Biodiesel – Produced from Rapeseed crops**
 - **100% pure, although is usually mixed with normal diesel for extra efficiency.**

(iii) increased CO₂ levels from combustion of fossil fuels leading to global warming and climate change (see also 2.4.1.d);

Burning Hydrocarbons increases atmospheric pollutants, such as

- **Carbon Monoxide – Toxic, formed by incomplete combustion,**
- **Carbon Dioxide – Contributes to global warming via greenhouse effect.**
- **Nitrogen Dioxides – Acid rain and destruction of forests.**
- **Sulfur Dioxide – Acid rain**

Greenhouse gases prevent heat escaping the atmosphere, leading to global temperature increase.

This may lead to heavier rainfall or frequent storms, or the opposite which may lead to melting of ice caps ---> this causes increased sea levels and floods and would call for a change of lifestyle for most of the worlds inhabitants.

(k) describe the substitution of alkanes using ultraviolet radiation, by Cl₂ and by Br₂, to form halogenoalkanes;

Alkanes react with UV radiation or at temperatures of about 300 °C.

Mechanism for Chlorination – CH₄ + Cl₂ -----> CH₃Cl + HCl

Initiation – Homolytic Fission

Cl₂ -----> Cl• + Cl•

Propagation

Step 1 . CH₄ + Cl• -----> •CH₃ + HCl

Step 2. •CH₃ + Cl₂-----> CH₃Cl + Cl•

Termination



(l) define the term radical as a **species with an unpaired electron**;

(m) describe how homolytic fission leads to the mechanism of radical substitution in alkanes in terms of initiation, propagation and termination reactions

When Homolytic fission occurs, each atom is left with an unpaired electron, so is now a free radical.

As atoms like to have a full outer shell, the radicals then react so that they can, leading to the radical substitution mechanism.

(n) explain the limitations of radical substitution in synthesis, arising from further substitution with formation of a mixture of products

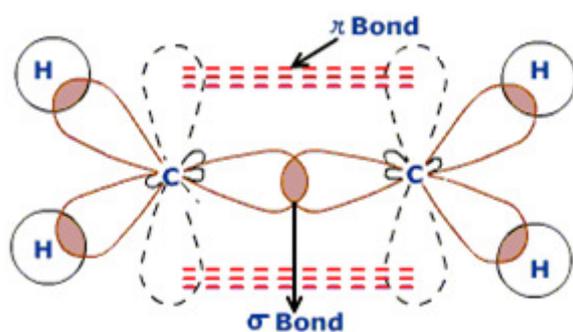
In synthesis, radical substitution is fairly inefficient.

In the termination steps, other organic products can form, so the product needed is not a 100% guarantee.

(a) state that alkenes **and cycloalkenes are unsaturated hydrocarbons**;

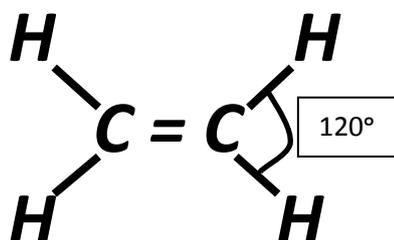
(b) describe the overlap of adjacent p-orbitals to form a π -bond;

A pi bond is formed by the overlapping of the p orbitals of two carbon atoms. Each carbon contributes one electron to the electron pair in a Pi bond (π bond). Sigma bonds (σ bonds) are formed by the overlapping of the s orbitals



(c) state and explain the trigonal planar shape around each carbon in the C=C of alkenes

Ethene is shaped as below:

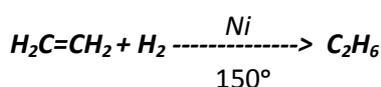


- There are 3 regions of electron density around each carbon.
- The pairs of electrons repel each other as far away as they can.
- Due to this, the double bond and the two single pairs produce a trigonal planar shape, with bond angles 120°

For the reactions below, see the sheet at the end on reactions for more detail.

(d) describe addition reactions of alkenes, ie by ethene and propene, with:

(i) hydrogen in the presence of a suitable catalyst, ie Ni, to form alkanes,



(ii) halogens to form dihalogenoalkanes, including the use of bromine to detect the presence of a double C=C bond as a test for unsaturation,

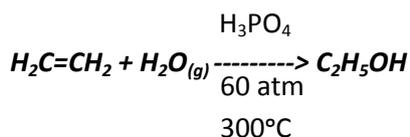


When bromine is added to a sample containing an Alkene, it turns from orange to colourless.

(iii) hydrogen halides to form halogenoalkanes,

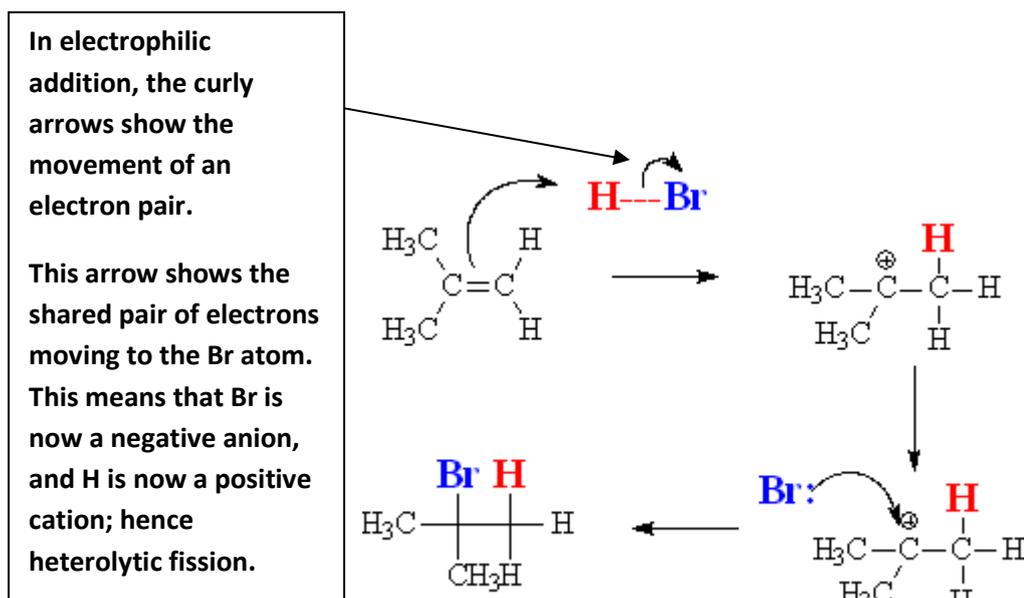
See Mechanism at end

(iv) steam in the presence of an acid catalyst to form alcohols;



(e) define an electrophile as an **electron pair acceptor**;

(f) describe how heterolytic fission leads to the mechanism of electrophilic addition in alkenes



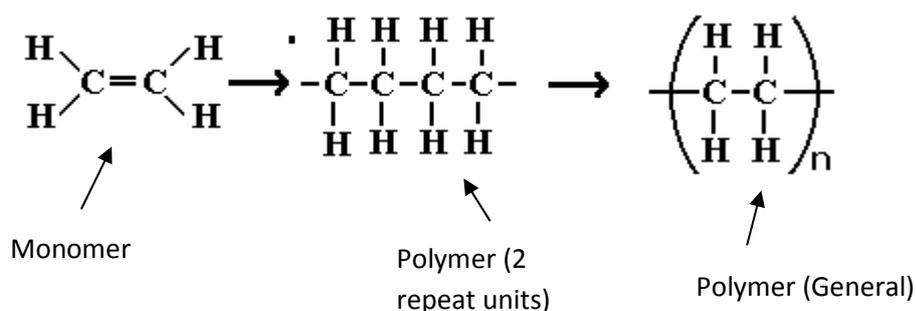
(g) describe the addition polymerisation of alkenes;

When Alkenes are polymerised, they go from their monomer form to their polymer form.

The monomer form is unsaturated and has a C=C bond.

The polymer is saturated, with only single bonds.

(h) deduce the repeat unit of an addition polymer obtained from a given monomer;



(j) outline the use of alkenes in the industrial production of organic compounds:

Alkenes may be used in order to form a number of industrial products, such as:

1. **1,2 – dichloroethane as a degreaser**
2. **Ethane – 1,2 –diol as antifreeze**
3. **Ethanoic acid as vinegar**
4. **Poly(tetrafluoroethene) as Teflon**

(i) **the manufacture of margarine by catalytic hydrogenation of unsaturated vegetable oils using hydrogen and a nickel catalyst**

(ii) *the formation of a range of polymers using unsaturated monomer units based on the ethene molecule, ie $H_2C=CHCl$, $F_2C=CF_2$;*

e.g

1. Ethene ($H_2C=CH_2$) ----> **Poly(ethene)**
2. Chloroethene ($HCIC=CHCl$) -----> **Poly(chloroethene) PVC**

(k) *outline the processing of waste polymers (see also 2.4.2) by:*

(i) **separation into types (ie PTFE, etc.) and recycling,**

(ii) **combustion for energy production**

(iii) *use as a feedstock for cracking in the production of plastics and other chemicals;*

(l) *outline the role of chemists in minimising environmental damage by:*

(i) **removal of toxic waste products, ie removal of HCl formed during disposal by combustion of halogenated plastics (ie PVC),**

PVC recycling plants have been opened in order to separate PVC from other scrap by dissolving it in solvents.

High quality PVC is then recovered by precipitation form the solvent. The solvent can be reused.

(ii) **development of biodegradable and compostable polymers, ie from isoprene (2-methyl-1,3-butadiene), maize and starch**

(a) *explain, in terms of hydrogen bonding, the water solubility and the relatively low volatility of alcohols;*

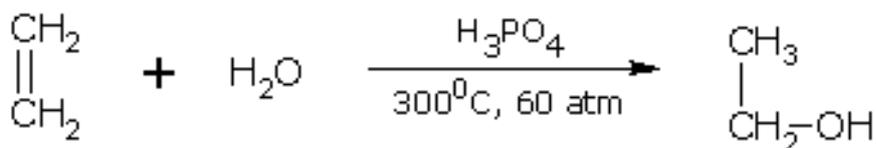
Due to alcohols having –OH groups attached to them, they have the ability to form hydrogen bonds, which are stronger than the van der Waals' forces that other alkanes/alkenes etc may have. This means that more energy is required to break it's bonds, meaning it has lower volatility. The hydrogen bond formation of alcohols, however, makes it easier for them to dissolve in polar products such as water.

(b) describe the industrial production of ethanol by:

(i) fermentation from sugars, ie from glucose,



(ii) the reaction of ethene with steam in the presence of an acid catalyst;



(c) outline, for alcohols:

(i) the use of **ethanol in alcoholic drinks and as a solvent in the form of methylated spirits**,

Ethanol may also be used as a fuel, blended with petroleum is burn more cleanly. It may also be used as methanol, which is another clean burning fuel used in racing cars. It is also an important feed stock in chemical industry.

(d) classify alcohols into primary, secondary and tertiary alcohols;

Primary Alcohol – The –OH group is attached to a carbon with 1 or no methyl group attached.

Secondary Alcohol - The –OH group is attached to a carbon with 2 methyl groups attached.

Tertiary Alcohol - The –OH group is attached to a carbon with 3 methyl groups attached.

(e) describe the combustion of alcohols;

Alcohols are combusted by oxidation.

An Alcohol is combusted completely is oxidised in an excess of Oxygen. It forms Carbon dioxide and water if this occurs.

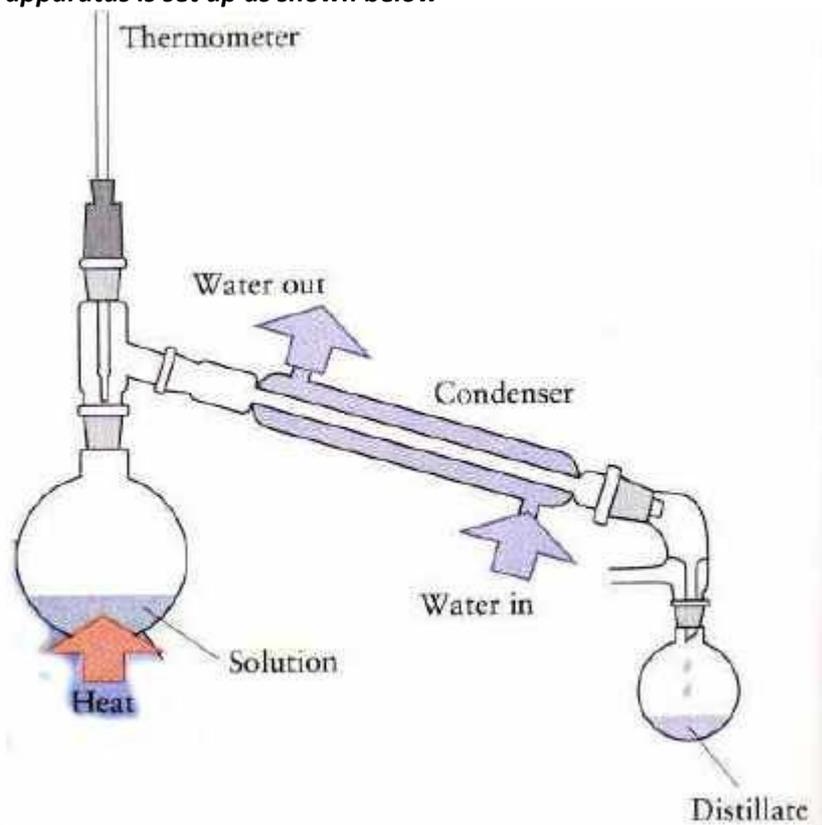
An Alcohol is combusted incompletely is oxidised when there is a shortage of oxygen. It forms Carbon monoxide and water.

(f) describe the oxidation of alcohols using $\text{Cr}_2\text{O}_7^{2-}/\text{H}^+$ (ie $\text{K}_2\text{Cr}_2\text{O}_7/\text{H}_2\text{SO}_4$), including:

(i) the oxidation of primary alcohols to form: aldehydes carboxylic acids; the control of the oxidation product using different reaction conditions,

Aldehydes:

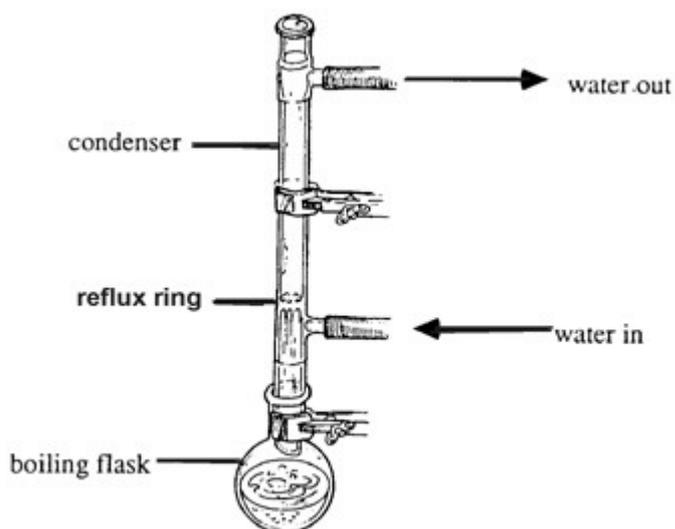
When a primary alcohol is oxidised, it is heated gently and then distilled to form an aldehyde. The apparatus is set up as shown below



If the condenser is set up the wrong way around, the vapour is not cooled properly, and this distillate collected may not be the desired aldehyde.

Carboxylic acids;

For a Carboxylic acid, a primary alcohol is heated under reflux.



The top of the tube is blocked so that the volatile liquid or gas cannot escape. It is not distilled so that the alcohol can be continually heated and oxidised so that eventually, a Carboxylic acid is formed.

(ii) the oxidation of secondary alcohols to form ketones,

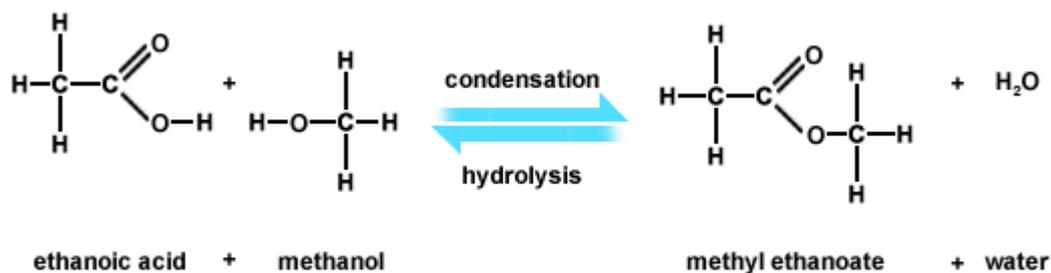
Secondary alcohols can only be processed into Ketones, they are simply heated.

(iii) the resistance to oxidation of tertiary alcohols;

Tertiary alcohols are resistant to oxidation. This is because there are no hydrogen atoms attached to the carbon of the OH group, so nothing forms on the chain.

(g) describe the esterification of alcohols with carboxylic acids in the presence of an acid catalyst;

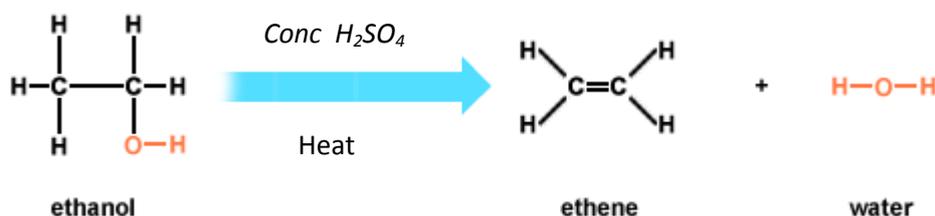
Esterification occurs when a Carboxylic acid is reacted with an alcohol in the presence of an Acid catalyst.



The OH from the carboxylic acid is removed, as well as the H from the alcohol. The C from the Carboxylic acid then joins to the O of the alcohol.

(h) describe elimination of H₂O from alcohols in the presence of an acid catalyst and heat to form alkenes.

When heated with Concentrated H₂SO₄, The OH group and an H is removed from an Alcohol to form an Alkene + H₂O



(a) describe the **hydrolysis of halogenoalkanes as a substitution reaction**;

(b) define the term nucleophile **as an electron pair donor**;

(c) describe the mechanism of nucleophilic substitution in the hydrolysis of primary halogenoalkanes with hot aqueous alkali (*see mechanisms*);

(d) explain the rates of hydrolysis of primary halogenoalkanes in terms of the relative bond enthalpies of carbon–halogen bonds (C–F, C–Cl, C–Br and C–I);

The rate of hydrolysis of haloalkanes depends on the bond enthalpy. Fluorine has the highest bond enthalpy so the rate of hydrolysis of it is therefore going to be slow.

The bond enthalpy decreases down the group, so as you go down the group 7, the rate of hydrolysis increases.

(e) outline the uses of chloroethene and tetrafluoroethene to produce the plastics PVC and PTFE (see also 2.1.3.g–i);

Chloroethene is polymerised to form Poly(chloroethene), is may be used in drainpipes, sports equipment and children’s toys.

Tetrafluoroethene forms Poly(tetrafluoroethene). The Carbon-fluorine bonds are very strong so they are inert and resistant to chemical attack. Along with its heat resistance and electrical insulating properties, it can be used to line pans and metal surfaces. It may also be used as nail polish.

(f) explain that CFCs:

(i) were developed as aerosols, refrigerants, and in air-conditioning and non-toxicity,

CFC’s are non flammable and non toxic so were appropriate for uses in fridges etc.

(ii) have caused environmental damage to the ozone layer (see also 2.4.1.g);

CFC’s break down in the presence of UV to form chlorine radicals which catalyse the breakdown of Ozone.

Ozone absorbs most UV, so an increasing amount of UV, especially UV-B causes an increase in global temperature and the number of skin related diseases such as Skin Cancer.

(g) outline the role of green chemistry in minimising damage to the environment by promoting biodegradable alternatives to CFCs, such as hydrocarbons and HCFCs; CO₂ as a blowing agent for expanded polymers (see also 2.4.2).

Hydrofluorocarbons (HFC’s) are now being used as alternatives to CFC’s, they still deplete the ozone later, however the depleting effect is about 1/10 of that of CFC’s.

HFC’s are only a short term replacement.

(a) state that **absorption of infrared radiation causes covalent bonds to vibrate;**

(b) identify, using an infrared spectrum of an organic compound:

(i) an alcohol from an absorption peak of the O–H bond,

The following peaks symbolise an OH bond

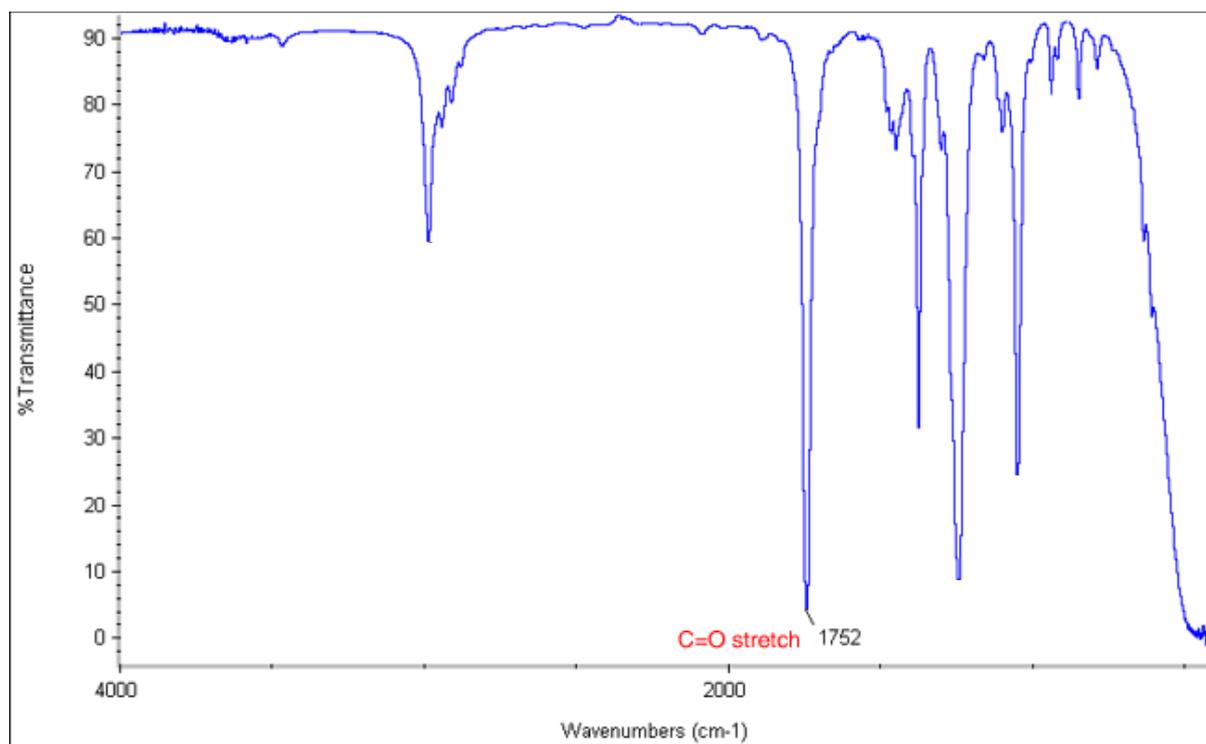
A very broad peak between 2500–3300 symbolises a carboxylic acid

A broad peak between 3200–3550 symbolises an alcohol

(ii) an aldehyde or ketone from an absorption peak of the C=O bond,

A peak between 1640-1750 symbolises a Aldehyde, Ketone, Carboxylic Acid or an Ester

e.g.



(iii) a carboxylic acid from an absorption peak of the C=O bond and a broad absorption peak of the O-H bond;

A peak between 1640-1750 and a broad peak between 2500-3300 symbolises a Carboxylic Acid

(c) state that **modern breathalysers measure ethanol in the breath by analysis using infrared spectroscopy;**

(d) outline the use of mass spectrometry:
(i) in the determination of relative isotopic masses,

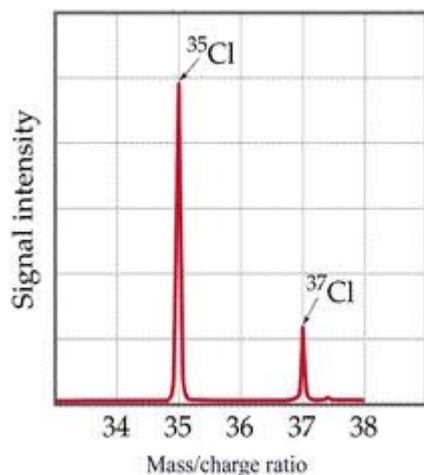
To identify the relative isotopic mass,

1. a substance is inserted into the spectrometer,
2. the molecules are then converted into ions.
3. Ions are propelled into a mass analyser
4. Ions are separated according to their mass to charge ratio.
5. Ions are detected and a mass spectrum is generated

(ii) as a method for identifying elements, ie use in the Mars space probe and in monitoring levels of environmental pollution, such as lead;

(e) interpret mass spectra of elements in terms of isotopic abundances;

A mass spectrum of Chlorine



Shows that relative abundance of each chlorine isotope.

(f) use the molecular ion peak in a mass spectrum of an organic molecule to determine its molecular mass;

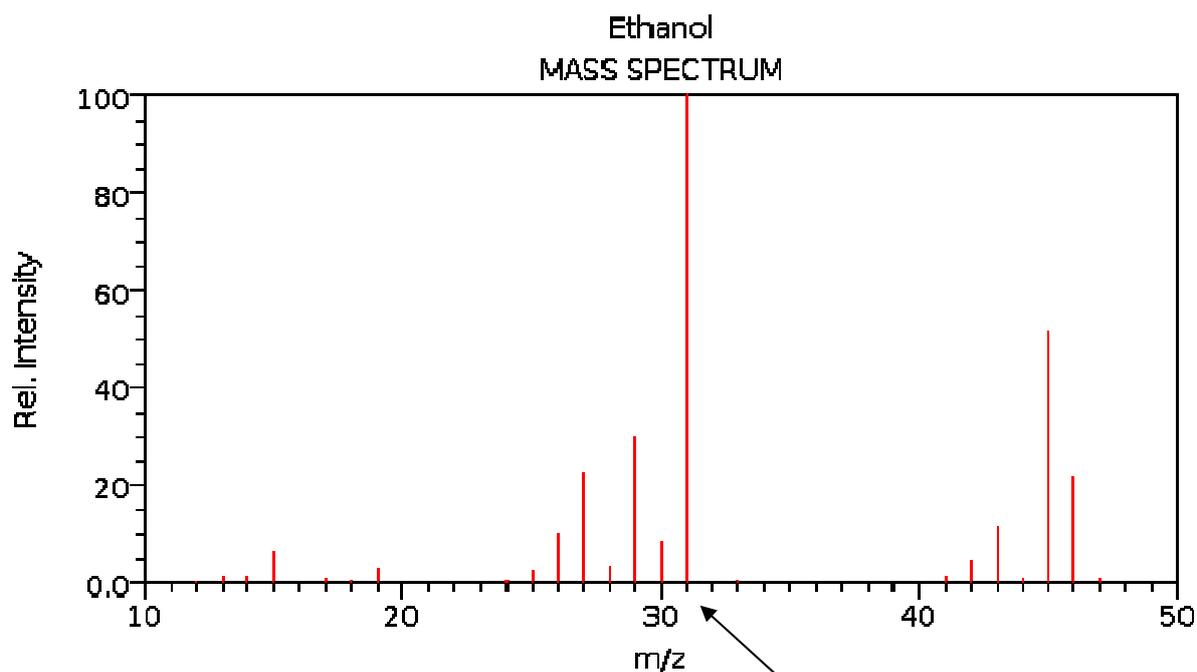
This is the same as calculating relative atomic mass.

**If the abundance of Chlorine – 35 is 84% and the abundance of Chlorine- 37 is 16%
(35 x 0.84) + (37 x 0.16) = 35.32**

(g) suggest the identity of the major fragment ions, ie $m/z = 29$ as CH_3CH_2^+ , in a given mass spectrum (limited to alkanes, alkenes and alcohols);

For the mass spectrum of Ethanol ($\text{C}_2\text{H}_5\text{OH}$)
We can see the peak at an M/Z of 46.
This is the fragment ion of $\text{C}_2\text{H}_5\text{OH}^+$ ←
A small peak can be seen at an M/Z of 47, this may be an isotope but it not the actual main peak.

When naming fragment ions, do NOT FORGET THE +



This peak for at 31, for example, can show that this has an OH group.

It shows the presence of a CH_2OH^+ fragment ion as the Mr of that value is $12+2+16+1 = 31$

(i) explain that **a mass spectrum is essentially a fingerprint for the molecule that can be identified by computer using a spectral database.**

(a) explain that **all chemical reactions are accompanied by enthalpy changes that can be exothermic (ΔH -ve) or endothermic (ΔH +ve);**

(b) describe **the importance of oxidation as an exothermic process in the combustion of fuels and the oxidation of carbohydrates such as glucose in respiration;**

Oxidation is the most exploited exothermic reaction.

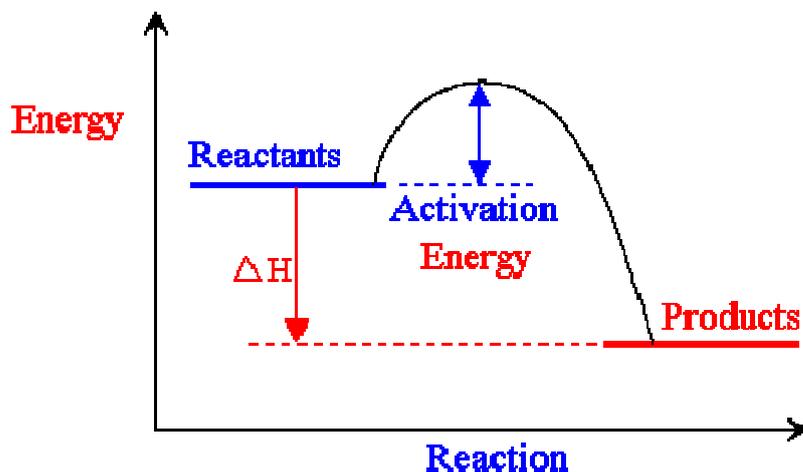
Combustion of fuels is the most common; we rely on it as our main source of energy. However, we now need to start considering alternatives due to our high carbon emissions and Global Warming.

(c) describe that **endothermic processes require an input of heat energy, e.g. the thermal decomposition of calcium carbonate;**

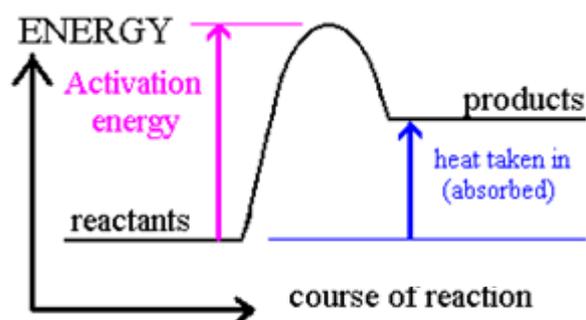
Endothermic reactions are Δ +ve as they require more energy to break the bonds than they do to form the bonds. Exothermic is vice versa.

(d) construct a simple enthalpy profile diagram for a reaction to show the difference in the enthalpy of the reactants compared with that of the products;

For an Exothermic Reaction



For an Endothermic reaction



(e) explain qualitatively, using enthalpy profile diagrams, the term activation energy;

The activation energy is the difference in energy between the reactants and the top of the energy curve. It shows the minimum energy required in order to start a reaction by breaking the bonds.

(f) define and use the terms:

(i) standard conditions,
100 kPa(Kilopascals) or 1 atmosphere
298K (Kelvin) or 25°C

(ii) enthalpy change of reaction,
The enthalpy change that occurs in a reaction, in the molar quantities expressed in a chemical equation under standard conditions, when all reactants and products are in their standard states.

(iii) enthalpy change of formation,
The enthalpy change when one mole of a compound is formed from its constituent elements in their standard states and conditions.

(iv) enthalpy change of combustion;
The enthalpy change when one mole of a substance is completely oxidised in an excess of oxygen under standard condition, with the reactants and products in their standard states.

(g) calculate enthalpy changes from appropriate experimental results directly, including use of the relationship: energy change = $mc\Delta T$;

$$Q=mc\Delta T$$

m - is the mass of the surroundings (The surroundings is the substance in which the thermometer is placed in)

c – The specific heat capacity (usually $4.18 \text{ Jg}^{-1}\text{K}^{-1}$)

ΔT – The change in temperature

When using this equation. If the temperature is increased, the reaction is exothermic, so the final answer must have a negative sign placed in front of it. And vice versa if the temperature decreases.

You must then calculate the number of moles of the surroundings.

After this, divide the Q by the number of moles for the overall enthalpy change per mole.

(h) explain exothermic and endothermic reactions in terms of enthalpy changes associated with the breaking and making of chemical bonds;

**When breaking bonds, energy is required. This means bond breaking is endothermic
When bonds are formed, energy is released. So this is exothermic.**

(i) define and use the term average bond enthalpy (ΔH positive; bond breaking of one mole of bonds);

Average enthalpy change that takes place when 1 mol of a given type of bond is broken by homolytic fission whilst in its gaseous state.

(j) calculate an enthalpy change of reaction from average bond enthalpies;

To calculate the enthalpy change, ΔH , you must

- 1. Find the total sum of the bond enthalpies of bonds broken (left side of equation)**
- 2. Find the total sum of the bond enthalpies of bonds made (right side of equation)**
- 3. Sum of bonds broken – Sum of bonds made (left – right)**

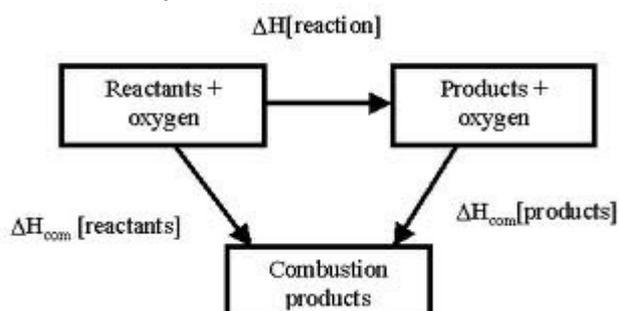
(k) use Hess' law to construct enthalpy cycles and carry out calculations to determine:

(i) an enthalpy change of reaction from enthalpy changes of combustion,

When using Enthalpy change of combustion figures (ΔH_c°) figures, the formula:

$$\Delta H = \text{Sum of } \Delta H_c^\circ \text{ reactants} - \text{Sum of } \Delta H_c^\circ \text{ Products}$$

This can be expressed as:

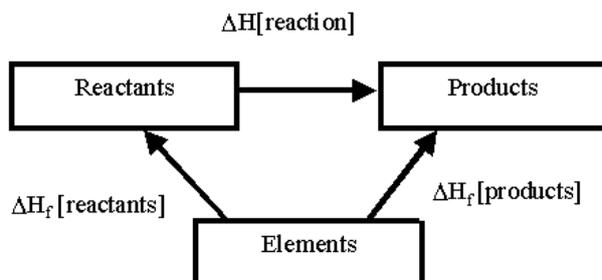


(ii) an enthalpy change of reaction from enthalpy changes of formation,

When using Enthalpy change of formation figures (ΔH_f°) figures, the formula:

$$\Delta H = \text{Sum of } \Delta H_f^\circ \text{ Products} - \text{Sum of } \Delta H_f^\circ \text{ reactants}$$

This can be expressed as:



(a) describe qualitatively, in terms of collision theory, the effect of concentration changes on the rate of a reaction;

Increasing the concentration:

1. **Makes the molecules closer together**
2. **Makes collisions more frequent and successful**
3. **Increase Rate of Reaction**

(b) explain why an increase in the pressure of a gas, increasing its concentration, may increase the rate of a reaction involving gases;

Increasing the pressure:

1. **The same number of molecules occupy a smaller space**
2. **More collisions will take place where the activation energy is met**
3. **Increases rate of reaction**

(c) state that **a catalyst speeds up a reaction without being consumed by the overall reaction;**

(d) explain that catalysts:

(i) affect the conditions that are needed, often **requiring lower temperatures and reducing energy demand and CO₂ emissions from burning of fossil fuels,**

(ii) enables different reactions to be used, with better atom economy and with reduced waste,

(iii) are often enzymes, generating very specific products and operating effectively close to room temperatures and pressures,

Such as detergents and washing powders

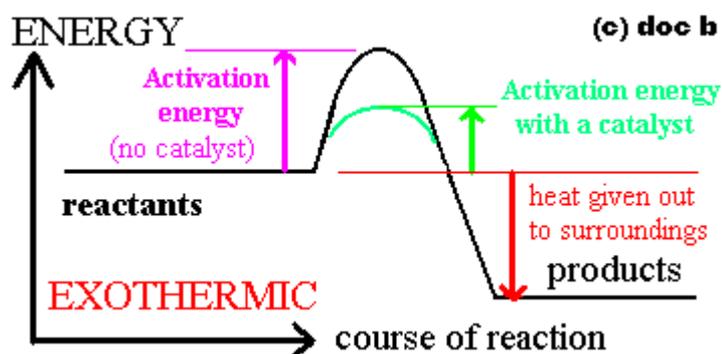
(iv) have great economic importance, eg iron in ammonia production, Ziegler–Natta catalyst in poly(ethene) production, platinum/palladium/rhodium in catalytic converters (see also 2.4.1.i);

Catalyst development leads to great profitability. Products are made more quickly, requiring less energy and creating less waste products.

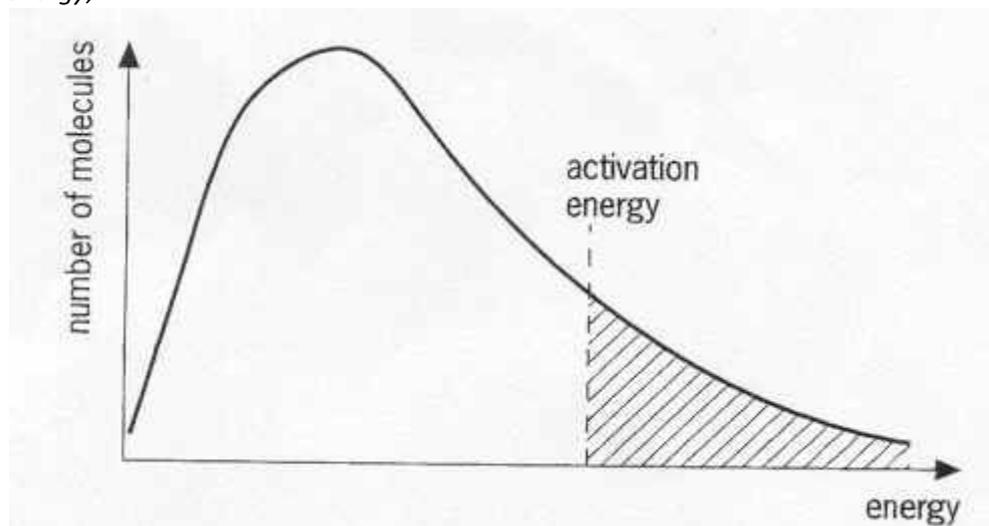
They may also be used in Catalytic converters found in cars, to convert toxic emissions into less harmful substances, such as CO_2 and N_2

(e) explain, using enthalpy profile diagrams, how the presence of a catalyst allows a reaction to proceed via a different route with a lower activation energy, giving rise to an increased reaction rate;

Catalysts may lower the activation energy of a reaction by offering an alternative pathway to the reaction.

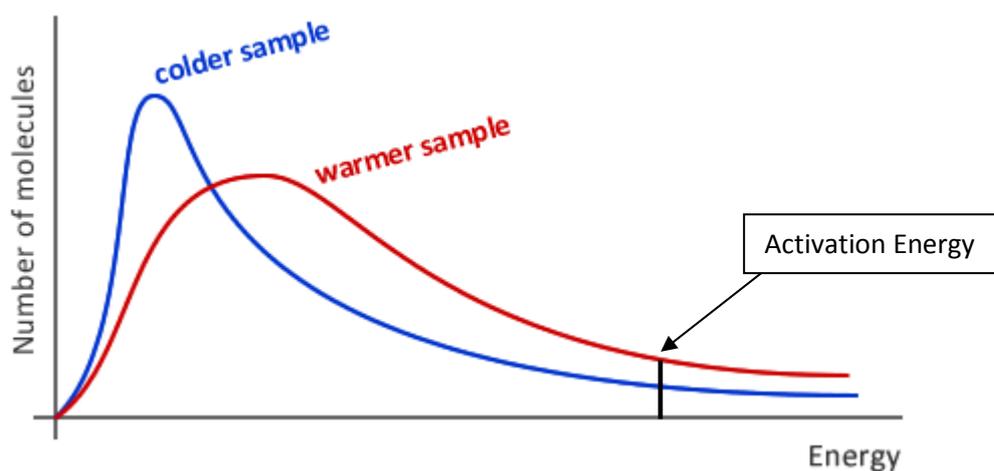


(f) explain qualitatively the Boltzmann distribution and its relationship with activation energy;



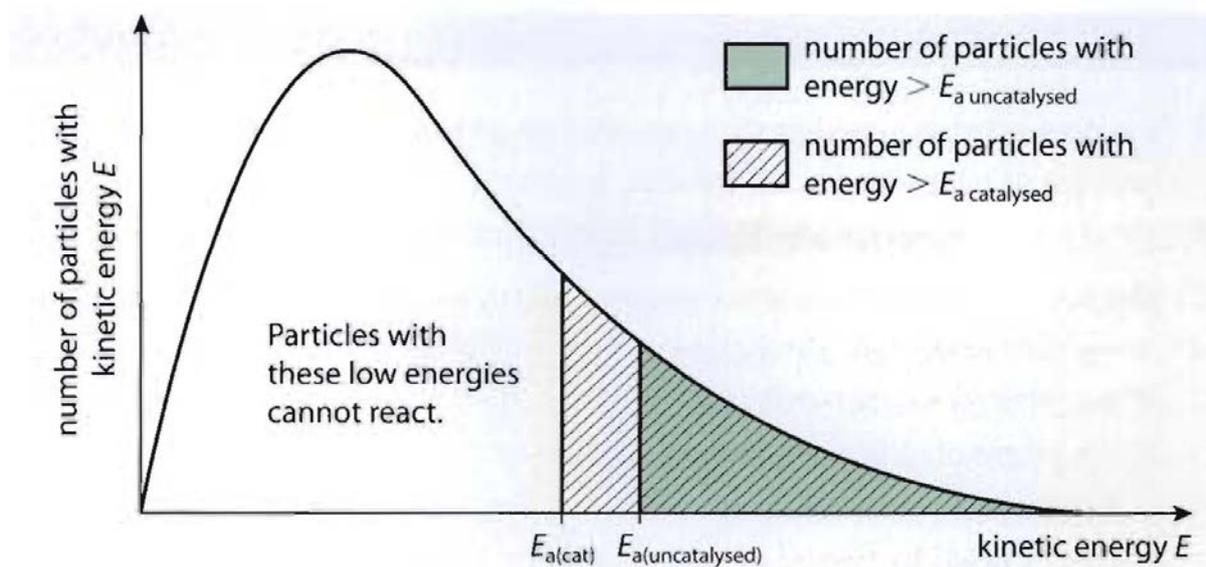
A Maxwell/Boltzmann distribution graph, shown above, shows the relationship between the number of molecules and the energy they possess during a reaction, The activation energy shows the point in which the energy must be exceeded in order for a collision to be successful. Only the molecules past the activation energy can cause the reaction to occur.

(g) describe qualitatively, using the Boltzmann distribution, the effect of temperature changes on the proportion of molecules exceeding the activation energy and hence the reaction rate;



This Boltzmann graph shows a warmer sample compared to a colder sample. The warmer sample has a high proportion of molecules with the required activation energy. This means that the warmer sample will undergo more successful, frequent collisions as more molecules have the required activation energy.

(h) interpret the catalytic behaviour in (e), in terms of the Boltzmann distribution;



Using a catalyst lowers the activation energy, this means that more molecules have the required activation energy so this, again, causes more frequent and successful collisions to occur.

(i) explain that a **dynamic equilibrium exists when the rate of the forward reaction is equal to the rate of the reverse reaction;**

(j) state le Chatelier's principle;

When a system is in dynamic equilibrium and is subjected to a change, the position of equilibrium will shift to minimise the change.

(k) apply le Chatelier's principle to deduce qualitatively (from appropriate information) the effect of a change in temperature, concentration or pressure, on a homogeneous system in equilibrium;

Temperature:

- 1. Increasing the temperature causes the position to move to the side that will decrease the temperature, so it moves to the left (+ve direction)**
- 2. Decreasing the temperature causes the position to increase the temperature, so moves to the right (-ve)**

Pressure:

- 1. Increasing the pressure causes the position of equilibrium to shift to the side with the fewer total of gas moles.**
- 2. Decreasing the pressure favours the side with the most moles of gas.**

Concentration:

1. **Of the Reactant:**
 - a. **Increasing the Concentration of the reactant moves the position to decrease the reactant concentration, so moves to the right.**
 - b. **Decreasing the Concentration of the reactant causes the equilibrium to try to increase the concentration, so the position moves to the left.**
2. **Of a Products**
 - a. **Increasing the Concentration of the product moves the position to decrease the product concentration, so moves to the left.**
 - b. **Decreasing the Concentration of the product causes the equilibrium to try to increase the concentration, so the position moves to the right.**

(l) explain, from given data, the importance in the chemical industry of a compromise between chemical equilibrium and reaction rate

Usually, optimum conditions of a reaction do not produce yield at the fastest rates. Industries must be able to produce a high yield in a respectable time in order to have a business, so these conditions are often compromised.

In the Haber process:

1. **The temperature must be high enough to produce a good enough yield rapidly, so 400°C is used.**
2. **Pressure – The pressure must not be too high as it would endanger the work force, so 200 atmospheres is used.**
3. **An iron catalyst is used to decrease the amount of energy needed and to also increase the rate of reaction by decreasing the cost also.**

(a) explain that infrared radiation is absorbed by C=O, O–H and C–H bonds in H₂O, CO₂ and CH₄, and that these absorptions contribute to global warming;

When IR is absorbed, the bonds emit this absorbed energy as radiation which may be absorbed by other greenhouse gas molecules or the Earth's surface.

(b) explain that the 'Greenhouse Effect' of a given gas is dependent both on its atmospheric concentration and its ability to absorb infrared radiation;

This is why CO₂ is such a big problem, it's extremely high concentration and its ability to readily absorb IR makes it a problem

(c) outline the importance of controlling global warming resulting from atmospheric increases in greenhouse gases;

It is important for us to control global warming.

In the Arctic, ice and permafrost is melting, Tropical areas are experiencing more frequent and destructive storms and floods. Glaciers are also disappearing.

The problems this causes include:

- 1. More flooding due to higher sea levels.**
- 2. Longer growing seasons for some, but drought and disease for others.**
- 3. Sea ice is melting, which may lead to severe winters in the UK**

(d) outline the role of chemists in minimising climate change resulting from global warming by:

(i) **providing scientific evidence to governments to verify that global warming is taking place,**

(ii) **investigating solutions to environmental problems, such as carbon capture and storage, CCS, ie the removal of waste carbon dioxide as a liquid injected deep in the oceans, storage in deep geological formations, by reaction with metal oxides to form stable carbonate minerals,**

(iii) **monitoring progress against initiatives such as the Kyoto protocol;**

(e) **explain that ozone is continuously being formed and broken down in the stratosphere by the action of ultraviolet radiation;**

(f) using the chemical equilibrium, below:
 $O_2 + O \rightleftharpoons O_3$

(i) describe and explain how the concentration of ozone is maintained in the ozone layer, including the role of ultraviolet radiation,

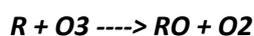
$O_3 + UV \text{ radiation} \rightleftharpoons O_2 + O$

$O_2 + O \rightleftharpoons O_3 + \text{heat}$

*(ii) outline the **role of ozone in the absorption of harmful ultraviolet radiation and the essential benefit of this process for life on Earth;***

Although Ozone prevents harm from Uv-B rays to our skin, low ozone can also be an air pollutant which can cause respiratory problems.

(g) understand that radicals, eg from CFCs, and NOx from thunderstorms or aircraft, may catalyse the breakdown of ozone by the following simple representation:



where R represents Cl• from a CFC or NO from nitrogen oxides;

(h) for carbon monoxide, oxides of nitrogen and unburnt hydrocarbons:

(i) explain their formation from the internal combustion engine,

Carbon Monoxide is released from car exhausts during incomplete combustion of fuel.

Oxides of Nitrogen form when air is drawn into the cylinder along with the fuel, the fuel is burned at high temperature and the nitrogen is oxidised by the oxygen.

Volatile organic compounds (VOC's) are released in vehicle exhaust gases from unburnt fuels and are human carcinogens

(ii) state environmental concerns from their toxicity and contribution to low-level ozone and photochemical smog;

Concentrations of low level ozone often build up on humid sunny days when the air contains a lot of hydrocarbons and oxides of nitrogen.

Urban areas are more susceptible to this than other areas.

Infrared Spectroscopy can be used to monitor environmental pollution.

(i) outline how a catalytic converter decreases carbon monoxide and nitrogen monoxide emissions from internal combustion engines by:

- 1. First, the CO and NO diffuse over the surface of the catalytic converter.**
- 2. They are then adsorbed on to the catalytic converters surface,**
- 3. The activation energy is lowered and weak bonds form with the converter**
- 4. The chemical reaction then occurs**
- 5. CO₂ and N₂ are then desorbed from the catalytic converters surface;**

(j) outline the use of infrared spectroscopy in monitoring air pollution.

Infrared Spectroscopy can be used to identify certain functional groups in the pollutants. The spectrum can be matched to known pollutants.

The abundance of the pollutant can then be examined and then a plan can be executed in order to try and prevent the further occurrences of this pollutant.

(a) describe principles of chemical sustainability:

(i) using industrial processes that reduce or eliminate hazardous chemicals and which involve the use of fewer chemicals,

(ii) designing processes with a high atom economy that minimise the production of waste materials,

(iii) using renewable resources such as plant-based substances,

(iv) seeking alternative energy sources such as solar energy, rather than consuming finite resources such as fossil fuels that will eventually be exhausted,

(v) ensuring that any waste products produced are non-toxic, and can be recycled or biodegraded by being broken down into harmless substances in the environment;

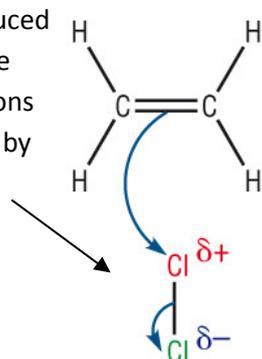
(c) explain the importance of establishing international cooperation to promote the reduction of pollution levels;

It is important to establish international co-operation as all countries contribute towards pollution. Atmospheric pollution also travels across borders. Co-operation between countries means that scientists can share ideas and theories about the causes and solutions to pollution; one country cannot control the total level of pollution unless all countries help.

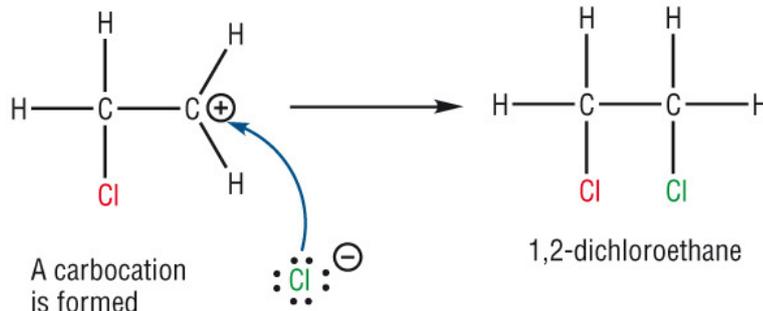
Mechanisms

Electrophilic Addition

A dipole is induced here due to the bonded electrons being repelled by the pi bond electrons

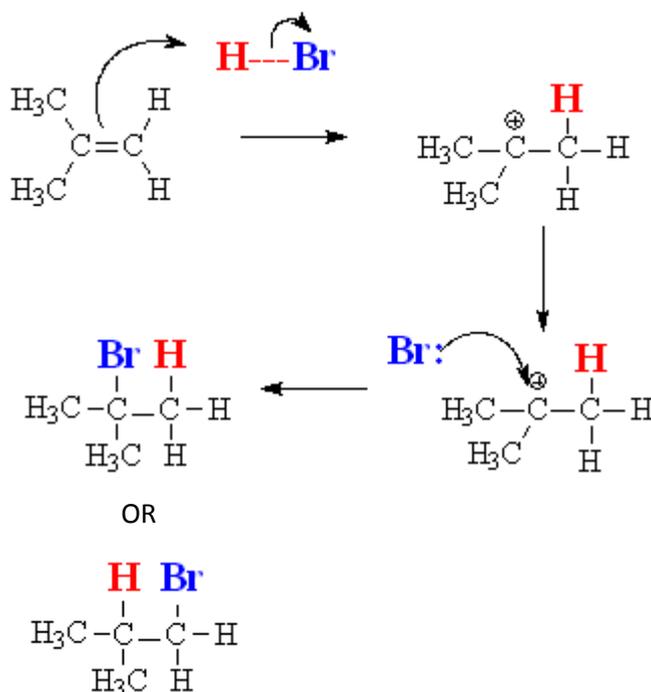


This carbon has a positive charge, so a carbocation is formed.



When Cl_2 approaches, the $\text{Cl}-\text{Cl}$ bond becomes polar. A pair of electrons flows from the double bond to the slightly positive $\text{Cl}^{\delta+}$ and a bond formed.

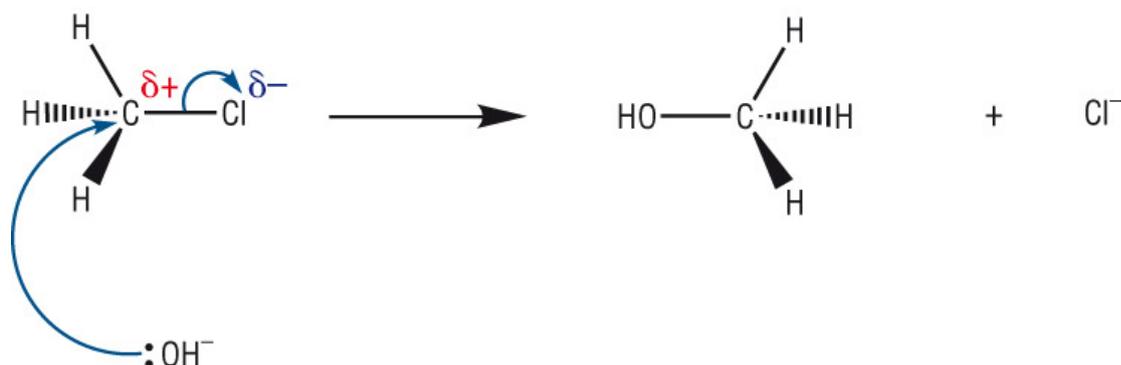
Also, addition of Hydrogen Halides



If an Alkene is unsymmetrical,
The H could end up being
bonded to either Carbon - 2 or
Carbon - 3.

The same could happen to the
BR

So this product could be either
2-bromopropane or 1-
bromopropane/

Nucleophilic Substitution

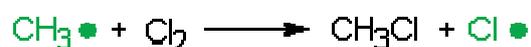
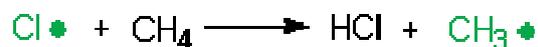
The nucleophile attacks the back of the carbon atom donating an electron pair. This causes a new bond to form and the carbon halogen bond to break.

Free Radical Substitution

1. Initiation reaction



2. Chain propagation



3. Chain termination reactions

