

OCR (B) Chemistry A-level

Storyline 2: Developing Fuels Detailed Notes

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Volumes of Gases

Molar Volume of Gases

One mole of any gas at **room temperature and pressure** will take up the **same volume**, regardless of its composition. This volume is 24,000 cm³, or 24 dm³, and is known as the **molar volume of gases**.

The Ideal Gas Law

When under **standard conditions**, gases and volatile liquids follow certain trends:

Pressure is proportional to Temperature
Volume is proportional to Temperature
Pressure and Volume are inversely proportional

These relationships can be combined to give the **ideal gas equation**:

$$pV = nRT = \frac{mRT}{M_r}$$

In order to use this equation, the variables must be in the correct **standard units**:

p = pressure in Pascals
V = volume in m³
T = temperature in Kelvin
n = moles
m = mass in grams

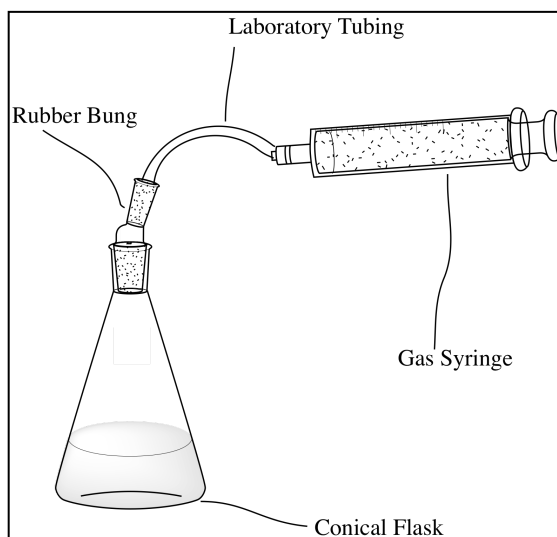
R is the **ideal gas constant**, equal to **8.31 JK⁻¹mol⁻¹**.

Experimental Techniques

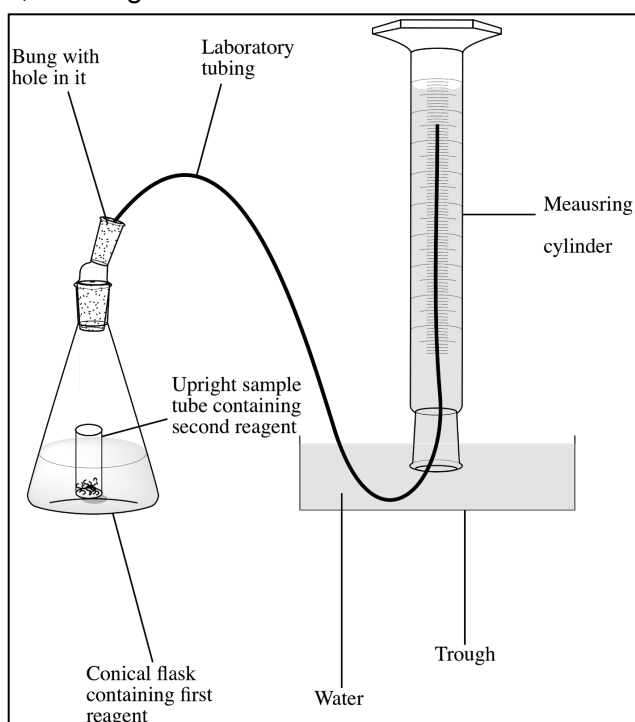
There are three main methods that can be used to measure the volume of gas released in an experiment.

1. Use a gas syringe to measure the volume of gas produced in an experiment.





2. Measure the mass lost on a weighing balance and calculate the moles of gas produced from this.
3. Collect the gas released from a reaction in an upturned test tube filled with water. The water is displaced by the gas, allowing its volume to be found.



Equations and Calculations

Full or ionic chemical equations must be **balanced** before they can be used in calculations. This is because the **reacting ratios** must be correct. For a chemical equation to be balanced, it must have the **same number and type** of each atom present on both sides of the equation.



It can be useful to also include **state symbols** so it is clear what might be observed during the reaction, for example, **bubbles** of gas, a **precipitate** forming, or a **colour change** that may infer a **displacement reaction**.

There are four state symbols:

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

Bonding and Structure

The Shapes of Simple Molecules and Ions

The shape of a simple molecule or ion is determined by the number of **electron pairs around the central atom** and the **repulsion** between them. Each electron pair **naturally repels** each other so that the **largest bond angle possible** exists between the covalent bonds.

In **diagrams**, a **solid line** indicates a bond that is in the plane of the paper, a **wedged line** indicates a bond that comes out of the plane of the paper and a **dotted line** indicates a bond that goes into the plane of the paper.

Bonding in Organic Molecules

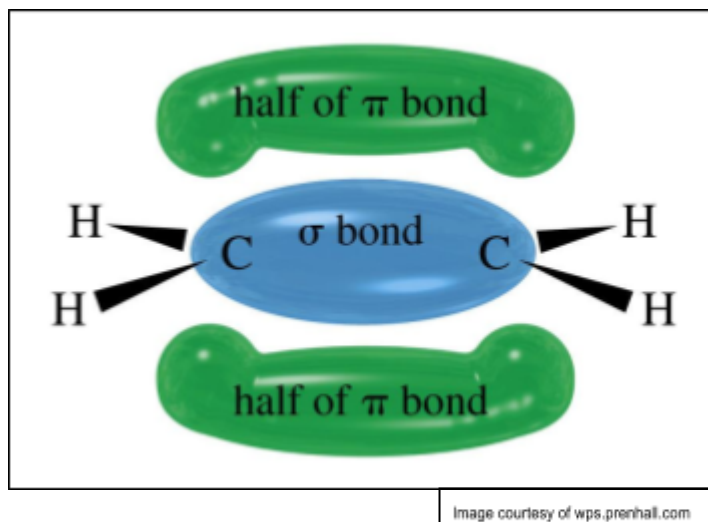
Organic molecules may contain single, double or triple bonds. Single bonds are called **σ bonds**. The overlap of orbitals is directly between the two atoms and there is **free rotation** around the σ bond.

Double bonds, such as carbon-carbon double bonds formed in alkenes, consist of a normal covalent **σ bond** and a **π bond**.

The **π -bond** is formed by **sideways overlap** of adjacent p-orbitals above and below the bonding atoms. The σ -bond is formed by overlap of orbitals directly between the bonding atoms.



Example:



Enthalpy Change (ΔH°)

Enthalpy change is heat energy change and is represented by the symbol ΔH° . Enthalpy is measured under standard conditions of **100 kPa pressure** and a specified temperature, generally **298 K**.

In a reaction, bonds are broken and then bonds are made. For bonds to be **broken**, energy is **taken in** from the surroundings, meaning bond breaking is an endothermic process. When bonds are **formed**, energy is **given out**, meaning bond making is an exothermic process. The overall energy change of the reaction depends on how much energy is transferred in these processes.

When energy is taken in from the surroundings, the **enthalpy change is positive**. When energy is released to the surroundings, the **enthalpy change is negative**.

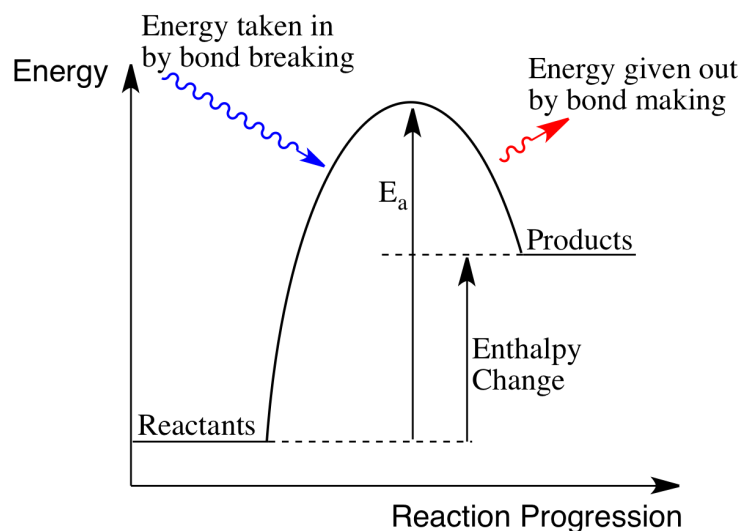
Overall enthalpy change (ΔH) can be calculated as follows:

$$\Delta H = \text{energy to break bonds (+ve)} + \text{energy to make bonds (-ve)}$$

Enthalpy changes in a reaction can be shown on an **energy level diagram**. These also indicate if the reaction is endothermic or exothermic.

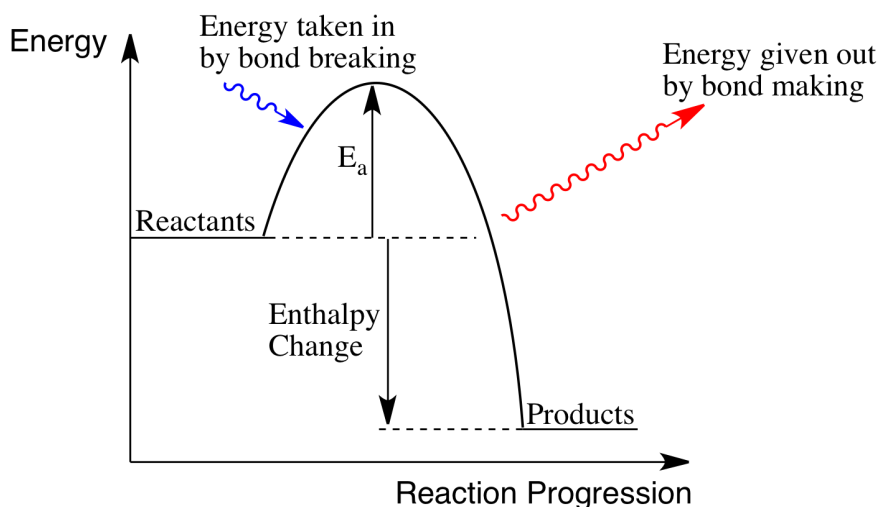


Example: Endothermic energy level diagram



In **endothermic** reactions more energy is needed to break bonds than make new ones. Therefore, the overall ΔH is **positive** and **heat is taken in** from the surroundings.

Example: Exothermic energy level diagram



In **exothermic** reactions the opposite is true, with more energy being needed to make new bonds than break existing ones. Therefore **heat is given out** and ΔH is **negative**.

Bond Enthalpies

Bond enthalpy data is an **averaged** value representing:

The energy required to break one mole of the stated bond in a gaseous state, under standard conditions.



Different covalent bonds require different amounts of energy to be broken. Values can be found experimentally using **calorimetry** methods. The bond enthalpy values calculated in this way often differ from the **data book values** as they are **not exact** and **vary in each situation**.

Mean bond enthalpy values tell you how much energy is required to break a particular bond, averaged out across the range of compounds containing that bond. These values relate to how **strong** a bond is, bonds with **lower** bond enthalpy values would be expected to break first.

The **shorter** a bond is, the **stronger** it is. **Double** and **triple** bonds are stronger than single bonds and have a shorter bond length.

Key Terms

Enthalpy Change of Reaction ($\Delta_r H^\circ$)

This is defined as:

The enthalpy change when quantities of substances in standard states react completely under standard conditions.

Enthalpy Change of Formation ($\Delta_f H^\circ$)

This is defined as:

The enthalpy change when one mole of a substance is produced from its elements under standard conditions.

Enthalpy Change of Combustion ($\Delta_c H^\circ$)

This is defined as:

The enthalpy change when one mole of a substance is burned completely in oxygen under standard conditions.

Enthalpy Change of Neutralisation ($\Delta_{\text{neut}} H^\circ$)

This is defined as:

The enthalpy change when solutions of acid and alkali react together under standard conditions to produce one mole of water.

Standard Conditions

This is defined as:

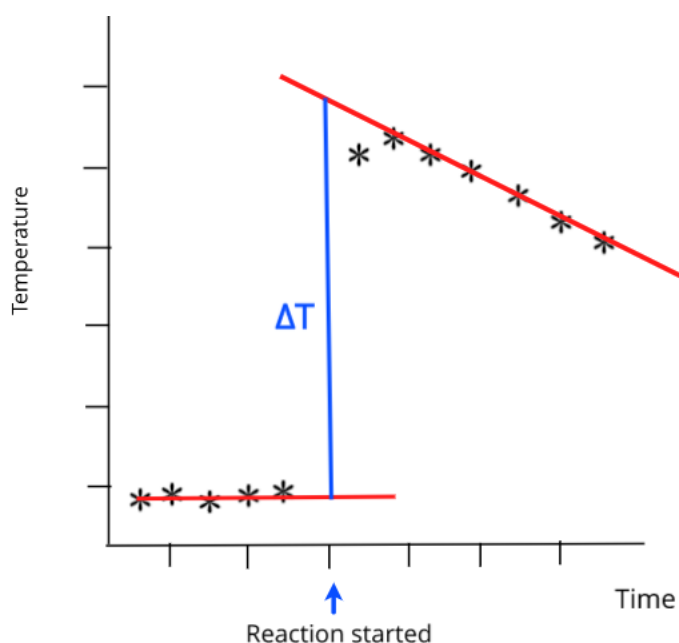
Solution concentrations of 1.00 mol dm⁻³, pressure 100 kPa and a stated temperature (generally 298K).



Calorimetry

Calorimetry is an **experimental method** for finding enthalpy change by measuring **temperature change over time** as a reaction occurs. When recorded and plotted on a graph, data can be **extrapolated** to give an accurate value for the change in temperature at the beginning of the reaction.

Example: Graph showing the extrapolated line of best fit



This measured change in temperature, ΔT , is **proportional** to the energy change:

$$q = mc\Delta T$$

(where q = energy change (J), m = mass (g), c = specific heat capacity ($\text{J g}^{-1} \text{ } ^\circ\text{C}^{-1}$), ΔT = temperature change ($^\circ\text{C}$))

This equation allows the energy change of a substance of known mass to be calculated. It depends on its **specific heat capacity**, defined as:

The energy required to raise 1g of the substance by 1K without a change of state.

Using this energy value (q), **enthalpy change per mole** (J mol^{-1}) of substance can be calculated:

$$\Delta H = \frac{q}{\text{moles}}$$

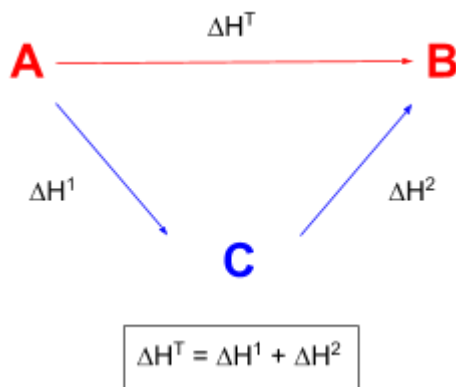


Hess's Law

Energy in a reaction system must be **conserved**, as it cannot be created or destroyed. Therefore, the **overall enthalpy change** for a reaction is **the same**, regardless of the **route taken**.

This is **Hess's Law** and it is used to determine the enthalpy changes for reactions that cannot be found directly using an experimental method. To do this, a **triangular cycle method** is used with an intermediate product. The direction of the arrows indicates whether the values should be added or taken away. They can be treated like vectors:

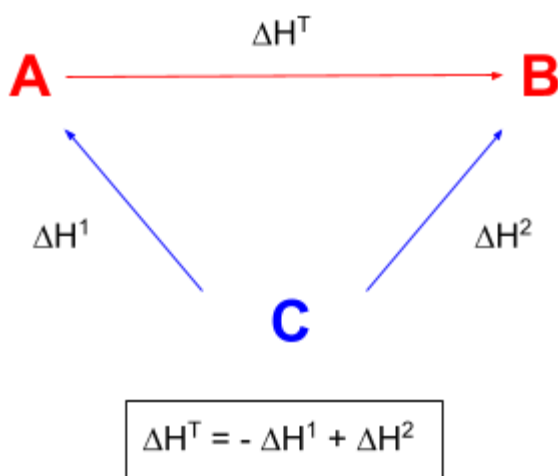
Example:



Enthalpies of Formation

Hess's law can be used to calculate an enthalpy change using given enthalpies of formation. When setting up the triangular diagram, the **arrows point up from the central product C** as both A and B are formed from the elements at C.

Example:



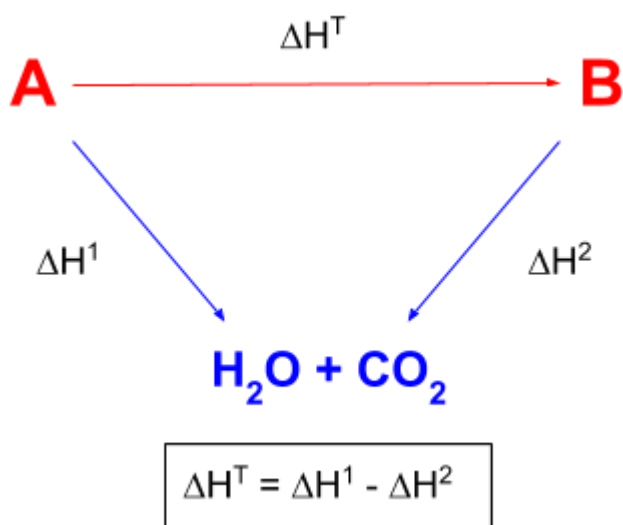
Note: ΔH^1 is subtracted as the reaction goes in the opposite direction to the arrow.

Enthalpies of Combustion

Hess's law can also be used to calculate an enthalpy change using given enthalpies of combustion. When setting up the triangular diagram, the **arrows point towards the central product (which is always H₂O and CO₂)** as both A and B burn to form the products at C.



Example:



Note: ΔH^2 is subtracted as the reaction goes in the opposite direction to the arrow.

Kinetics

Catalysts

Catalysts **lower the activation energy** (the minimum energy required for a reaction to occur) of a reaction by providing an **alternative reaction route**.

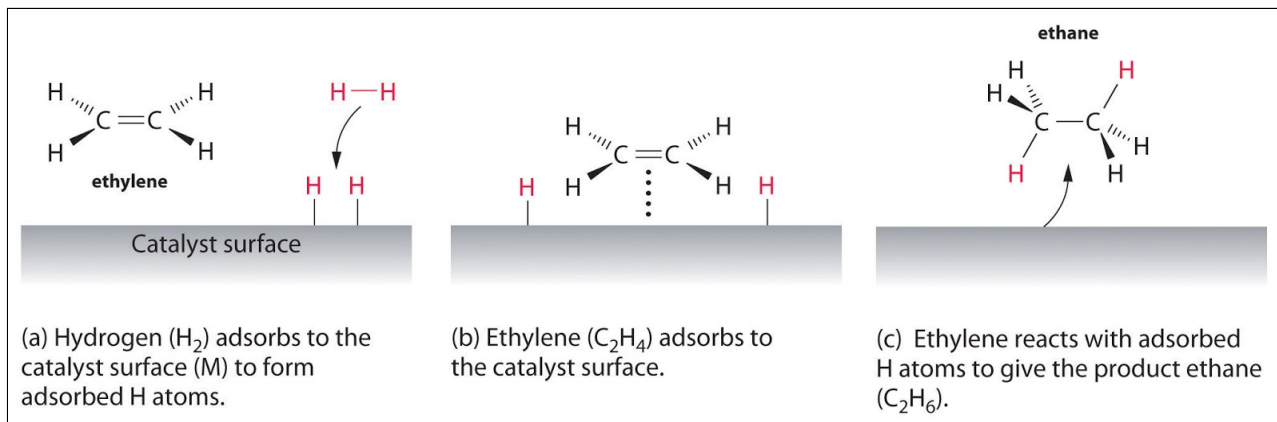
Heterogeneous Catalysts

Heterogeneous catalysts are catalysts that are in a **different phase or state** to the species in the reaction.

A solid heterogeneous catalyst works by **adsorbing** molecules onto an **active site** on the surface of the catalyst. These active sites **increase the proximity** of molecules and **weaken the covalent bonds** in the molecules, allowing reactions to occur more easily. This leads to a faster rate of reaction. These catalysts are used in **industry** to give a **surface** for the reaction to occur on.



Example:



Impurities in a reaction mixture may bind to a heterogeneous catalyst's **surface** and **block** reactants from being adsorbed. This is known as **catalyst poisoning** and it reduces the **activity** of the catalyst.

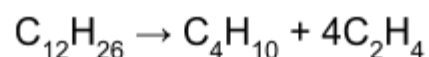
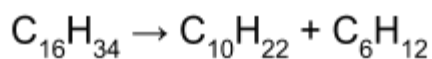
Cracking

Cracking is a process used to convert **long-chain** hydrocarbons into **shorter, more useful** hydrocarbons. The carbon-carbon bonds are broken in order to do this, which requires quite **harsh reaction conditions**. There are two main types of cracking which result in slightly different organic compounds.

Thermal cracking uses high temperatures and pressures.

Catalytic cracking produces **aromatic compounds** with carbon rings. Lower temperatures around **720 K** are used along with normal pressure, but a **catalyst** is also used to compensate for these less harsh conditions. The **hydrocarbon vapour** is passed over the **heated catalyst**.

Examples:



Combustion of Fuels

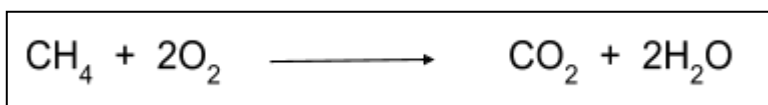
Fuels are combusted to release energy. During this, pollutants are released into the atmosphere. **Pollutants** are substances that have an undesired effect on the air, water or environment. There are, however, methods that help to reduce the release of these pollutants.

Hydrocarbons such as alkanes make good fuels as they **release a lot of energy** when burned. With sufficient oxygen present, they undergo **complete combustion** to produce carbon dioxide



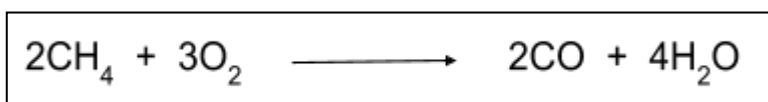
and water. Carbon dioxide is a **greenhouse gas** so causes **global warming** and contributes to **climate change**.

Example:



If the oxygen present is insufficient, combustion is **incomplete** and **carbon monoxide or carbon** is produced alongside water.

Example:



Carbon monoxide is a **toxic**, gaseous product which is especially dangerous to humans as it is odourless and colourless. Carbon monoxide is dangerous because it **replaces oxygen** in the blood, starves the brain and other organs of oxygen and causes **suffocation**.

Oxides of **nitrogen** and **sulfur** are also produced as byproducts of alkane combustion along with carbon particulates from unburnt fuel. In the clouds these oxides can react with water and form dilute acids, which result in **acid rain**. Acid rain can erode buildings and statues made from limestone and can make lakes and rivers **acidic**, killing wildlife.

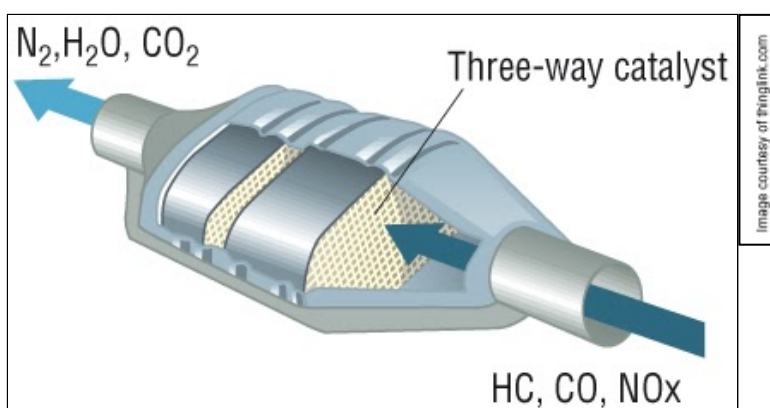
Carbon Particulates

Incomplete combustion can also produce **carbon particulates**, small fragments of unburned hydrocarbons. Unless removed from the waste products in industry, these can cause serious **respiratory problems** as they pollute the air. They also contribute to **global dimming**.

Catalytic Converters

Unburnt hydrocarbons and oxides of nitrogen can be removed from systems using a **catalytic converter**. This uses a **rhodium catalyst** to convert harmful products into more stable products such as CO_2 or H_2O .

Example:



Organic Chemistry

Hydrocarbons

Organic chemistry mainly concerns the properties and reactions of **hydrocarbons**, compounds that contain **only carbon and hydrogen** atoms. Hydrocarbons are a series of compounds with similar structures and formulas that can be represented in many different ways.

Nomenclature

Nomenclature is the set of rules that outline how different organic compounds should be **named** and how their **formulas are represented**.

Homologous Series

Organic compounds are often part of a **homologous series**, in which all members follow a **general formula** and react in a very similar way. Each consecutive member **differs by CH_2** and there is an **increase in boiling points** as chain length increases.

Example:

Image courtesy of DP Chemistry

Molecular Formula	Condensed Structural Formula	Name	Boiling Point (°C)
CH_4	CH_4	Methane	-161
C_2H_6	CH_3CH_3	Ethane	-89
C_3H_8	$\text{CH}_3\text{CH}_2\text{CH}_3$	Propane	-44
C_4H_{10}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	Butane	-0.5
C_5H_{12}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Pentane	36
C_6H_{14}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Hexane	68
C_7H_{16}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Heptane	98
C_8H_{18}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Octane	125
C_9H_{20}	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Nonane	151
$\text{C}_{10}\text{H}_{22}$	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	Decane	174

Each series has a **functional group** that allows that molecule to be recognised as being able to react chemically in a certain way as a result of that group.

Naming Compounds

Compounds are named according to rules laid out by the **International Union of Pure and Applied Chemistry (IUPAC)**. This ensures each compound is universally named the same - which helps to avoid potentially dangerous confusion.

As well as being able to name compounds from their structures, you should be able to draw structures from IUPAC names.



Stem

The prefix of the chemical tells you **the length of the longest unbroken chain of carbon atoms** in the compound. The first 10 are given below, using alkanes as an example:

Number of C atoms	Prefix	Alkane example
1	Meth-	Methane
2	Eth-	Ethane
3	Prop-	Propane
4	But-	Butane
5	Pent-	Pentane
6	Hex-	Hexane
7	Hept-	Heptane
8	Oct-	Octane
9	Non-	Nonane
10	Dec-	Decane

Functional Groups

The **ending** of the compound's name tells you the **functional group** present. If there is more than one functional group present, they are added as a **suffix**.

Functional group	Suffix
Alkane	-ane
Alkene	-ene
Alcohol	-ol

If a **halogen** is present, it is represented by a **prefix**:

Functional group	Prefix
Fluorine	Fluoro-
Chlorine	Chloro-
Bromine	Bromo-
Iodine	Iodo-

Side Chains

Carbon side chains that are **branches** from the longest carbon chain are represented by a **prefix** at the start of the word. These **alkyl groups** are made using the **stems** given above (meth-, eth-, prop-, etc) and the **suffix -yl**.



Organic compounds that contain branched or straight carbon chains (no rings) are known as **aliphatic compounds**.

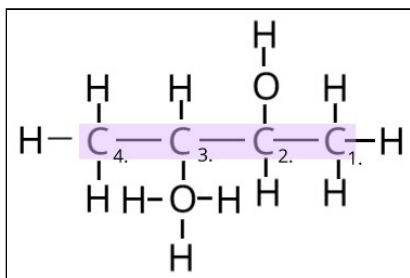
General Rules

1. Functional groups and side chains are given, if necessary, with the number corresponding to the carbon they are attached to.
2. Numbers are separated by commas.
3. Numbers and words are separated by hyphens.
4. If more than one particular side chain or functional group is present then one of the following prefixes is added: di- (2), tri- (3), tetra- (4), etc.
5. The carbon chain is numbered in ascending order from the end of the chain nearest a functional group.
6. If multiple prefixes are present, they are included in alphabetical order.

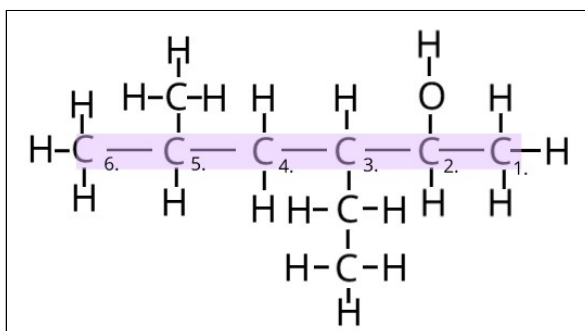
Examples

Example 1: The displayed structure of butan-2,3-diol.

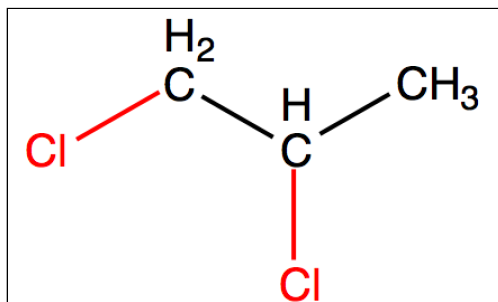
This compound only has single carbon-carbon bonds, so is an alkane. Its longest chain of carbon atoms is 4, giving the stem butan-, and it has two alcohol functional groups on carbons 2 and 3.



Example 2: The displayed structure of 3-ethyl,5-methylhexan-2-ol.



Example 3: The skeletal structure of 1,2-dichloropropane

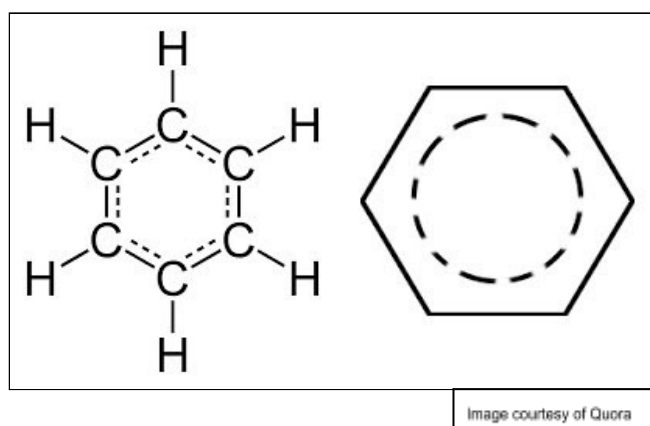


Aromatic Compounds

Arenes are aromatic compounds that **contain a benzene ring as part of their structure**.

Benzene consists of a ring of **six carbon atoms** each bonded to **one hydrogen atom**, giving it the molecular formula C_6H_6 . This structure means benzene has a ring of **delocalised electrons**:

Example: Displayed and skeletal formula of benzene



Saturated and Unsaturated Compounds

Alkanes are an example of a **saturated compound**. Saturated compounds only contain C-C single bonds.

Unsaturated compounds, on the other hand, are organic compounds that contains at least one C=C double bond, a $C\equiv C$ triple bond or an aromatic ring.

Organic Reactions of Alkenes

Introduction to Alkenes

Alkenes are **unsaturated hydrocarbons** with at least one carbon-carbon **double bond**. They are part of a homologous series with the general formula C_nH_{2n} .

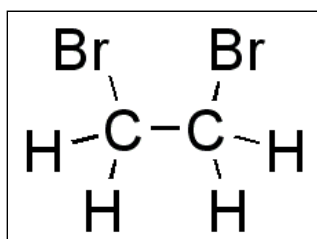


The carbon double bond is an area of **high electron density** making it susceptible to attack from electrophiles (species that are attracted to δ^- areas). This makes alkenes more reactive than alkanes.

Test for Alkenes

Bromine water is used to identify an alkene double bond and other unsaturated compounds. Alkenes cause bromine water to change colour from **orange-brown to colourless**. This is because the C=C bond can 'open up' to accept bromine atoms, and thus become saturated. The product of the reaction of alkenes with bromine is a dibromo compound.

Example:



Electrophilic Addition

Alkenes react with electrophiles and undergo **electrophilic addition** about the double bond.

Electrophiles are **electron acceptors** and are attracted to areas of high electron density. Some of the most common electrophiles are:

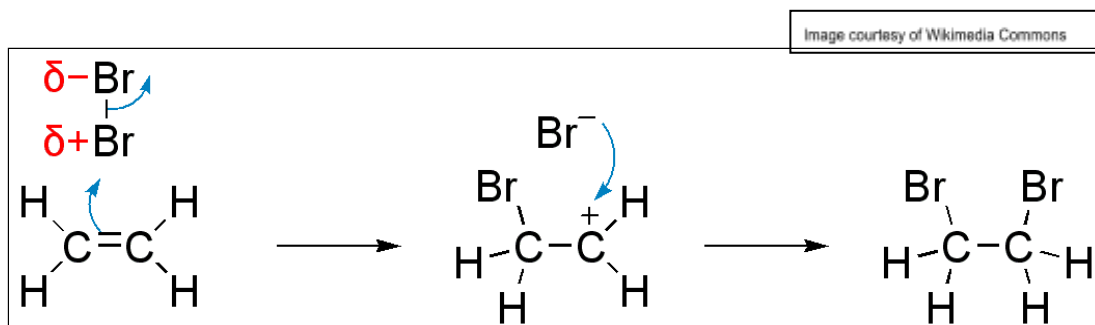
- HBr
- Br₂
- H₂SO₄

Electrophilic addition is the reaction mechanism that shows how electrophiles attack the double bond in alkenes. When the double bond is broken, a **carbocation** forms. This is a carbon atom with only **three bonds**, meaning it has a **positive** charge.

Alkenes can undergo addition reactions with a variety of molecules to give different products.

Curly arrows are used in mechanisms to show the movement of a pair of electrons.

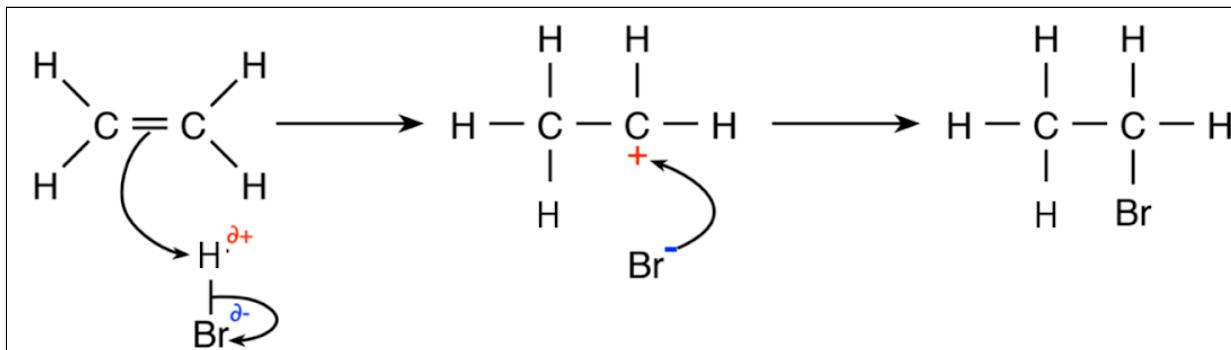
Mechanism: Alkene + Halogen → Dihalogenoalkane



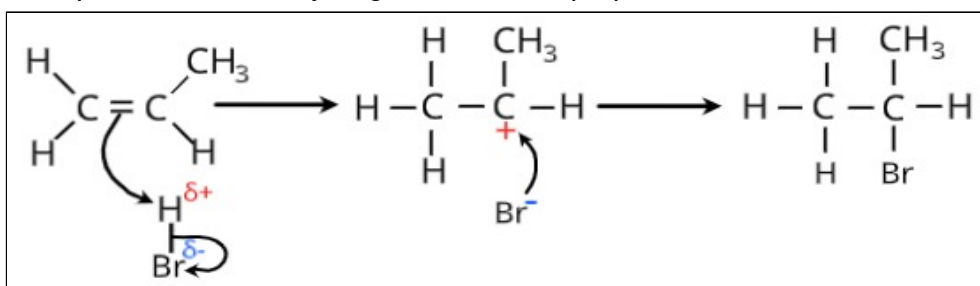
The π bond causes the bromine molecule to gain a temporary dipole so that electrons are transferred.

Mechanism: Alkene + Hydrogen Halide \rightarrow Halogenoalkane

Example: Electrophilic addition of hydrogen bromide to ethene



Example: Electrophilic addition of hydrogen bromide to propene



Alkenes undergo **addition reactions with hydrogen**, H_2 , in the presence of a catalyst to form alkanes. The conditions required for this reaction depends on the catalyst used:

- Nickel catalyst and high temperature and pressure.
- Platinum catalyst and room temperature and pressure.

Alkenes undergo **addition reactions with water**, H_2O , in the presence of a catalyst to form alcohols. The conditions required for this reaction depends on the catalyst used:

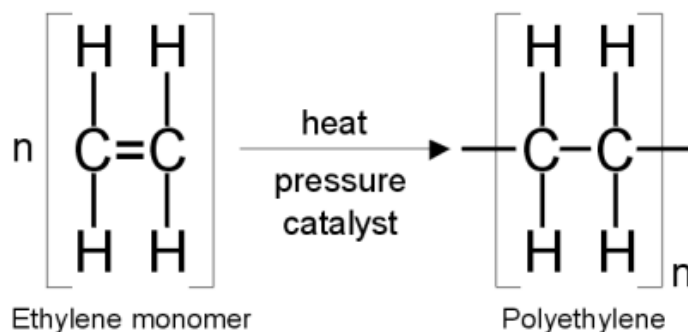
- Concentration sulfuric acid, H_2SO_4 , then add water
- Steam, phosphoric acid (H_3PO_4), high temperature and pressure

Addition Polymers

Addition polymers are produced from **alkenes**, where the double bond is broken to form a **repeating unit**. Alkenes are short chain **monomers** which join together to form **long chain** polymers.



Example:



The repeating unit must always be shown with **extended bonds through the brackets**, showing that it bonds to other repeating units on both sides.

Isomerism

Formulae

There are many different way of writing and representing organic compounds:

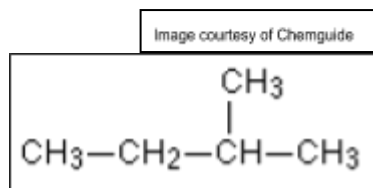
1. Molecular Formula

- The actual number of atoms of each element in a compound.

2. Structural Formula

- Shows the structural arrangement of atoms within a molecule.

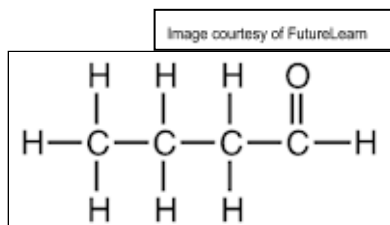
Example:



3. Displayed Formula

- Shows every atom and every bond in an organic compound.

Example:



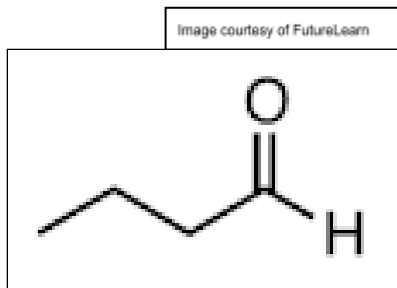
4. Skeletal Formula

- Shows only the bonds in a compound and any non-carbon atoms.
 - Vertices are carbon atoms.



- Hydrogen is assumed to be bonded to them unless stated otherwise.

Example:



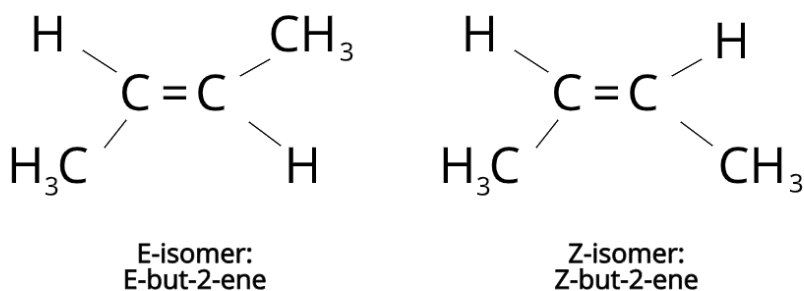
Stereoisomers

Stereoisomers have the same structural formula but have a **different spatial arrangement** of atoms and bonds.

E-Z isomerism is a type of stereoisomerism that arises in compounds with one hydrogen atom attached to each carbon atom on a C=C. This isomerism occurs due to the **limited rotation** around a double carbon bond. The limited rotation means that the hydrogen atoms attached to the C=C can either be 'together' or 'apart'.

The **E** isomer (german for 'entgegen' meaning apart) is when the hydrogen atoms are **apart**. The **Z** isomer (german for 'zusammen' meaning together) has the hydrogen atoms **together** on the same side.

Example:



Cis- and Trans- isomers

Stereoisomers can be named in the same process as above, but instead using **Cis-** for when the groups are on the **same side** and **trans-** for when they are **different sides**. Cis- and trans- differs from E/Z isomerism in that cis- and trans- can only be used when one of the groups on each carbon atoms is the same, giving something to compare the two other groups to.



Sustainability

Earlier in this topic, some of the environmental problems associated with the burning of fuels were outlined. Alternative fuels are now being developed such as **biofuels** that release fewer, less harmful products when burned.

Ethanol is a common **biofuel**. It is said to be **carbon neutral** as the carbon given out when it is burned is equal to the carbon taken in by the crops during the growing process. Hydrogen is another carbon neutral fuel, as the only product of its combustion is water.

The other advantage to biofuels is that they are **sustainable**. This means their supply can be maintained at the rate it is being used, so they will not run-out - unlike **fossil fuels**.

