Edexcel IAL Chemistry A-Level

Topic 4: Introductory Organic Chemistry and Alkanes

Detailed Notes

Topic 4A: Introduction

Hazards and Risks

Introduction

Hazards and **risks** are not the same. A hazard is anything that could **cause harm** while a risk is the **likelihood** of that hazard causing harm. In the context of chemistry, hazards could be things like inhalation of, spillage of, or contact with **harmful chemicals,** or breaking **glassware**.

Possible **hazardous properties** associated with organic compounds:

- **Flammable** - easily ignites.
- **Volatile** - has a low boiling point so readily evaporates at temperatures used in common lab experiments.
- **Toxic** - can cause damage to an organism.
- **Corrosive** - can cause damage to living tissue.

Risk assessment

When working with hazardous chemicals it is important to carry out a **risk assessment**. This involves identifying the possible hazards in an experiment and planning how to **reduce or eliminate the risk** of that hazard.

Reducing risk

Risk can be **reduced** by **planning** action against the hazards associated with each step in an experiment. There are some more general ways the risk can be reduced. For example, carrying out the experiment on a **smaller scale** or using a **different chemical** or piece of equipment in the place of a more hazardous one are both actions which will reduce risk.

Hydrocarbons

Organic chemistry mainly concerns the properties and reactions of **hydrocarbons**, compounds that contain **only carbon and hydrogen** atoms. Hydrocarbons form 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**.

Formulas

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

1. **Empirical Formula**
   - The simplest whole number ratio of atoms of each element in a compound.

2. **Molecular Formula**
   - The actual number of atoms of each element in a compound.

3. **General Formula**
   - All members of a homologous organic series follow the general formula.

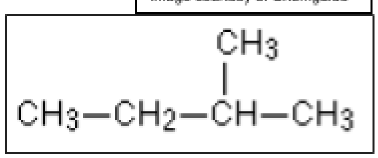
   Example:

   $$\text{Alkanes} = C_nH_{2n+2}$$

4. **Structural Formula**
   - Shows the structural arrangement of atoms within a molecule.

   Example:

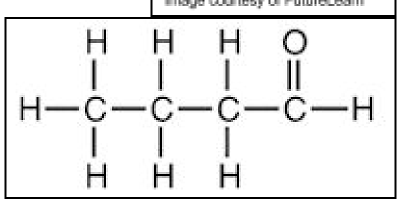
   Image courtesy of Chemguide



5. **Displayed Formula**
   - Shows every atom and every bond in an organic compound.

   Example:

   Image courtesy of FutureLearn

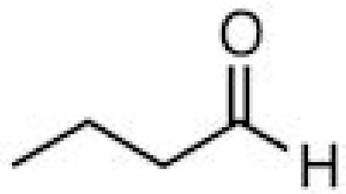


6. **Skeletal Formula**
   - Shows only the bonds in a compound and any non-carbon atoms.
   - Vertices are carbon atoms.

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

Example:

Image courtesy of FutureLearn

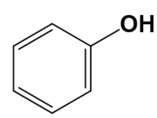
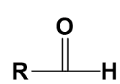
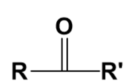
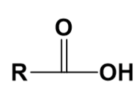
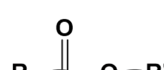


Homologous Series

Organic compounds are generally 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.

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

Example: Table of functional groups (ignore ethers)

Name	Functional Group	IUPAC Ending
Alcohols	R—OH	-ol
Phenols		phenol
Ethers	R—O—R'	ether
Aldehydes		-al
Ketones		-one
Carboxylic Acids		-oic acid
Esters		-ate

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 **prefix**.

Functional group	Suffix
Alkane	-ane
Alkene	-ene
Alcohol	-ol
Carboxylic acid	-oic acid
Ketone	-one
Aldehyde	-al
Ester	-ate
Amine	-amine

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.**

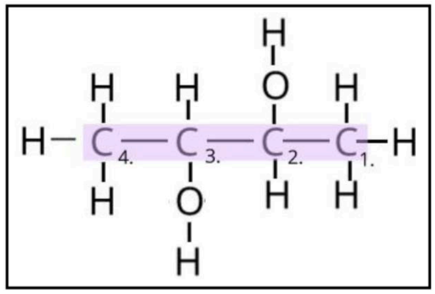
General rules

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.

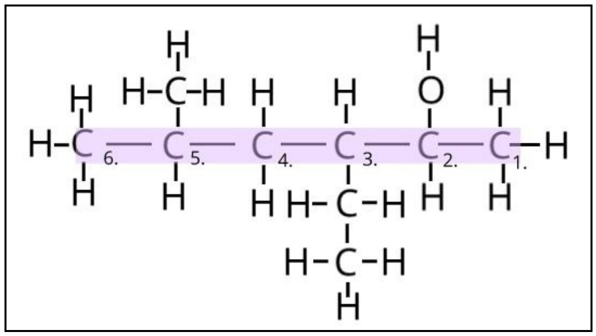
Examples

Example: 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.

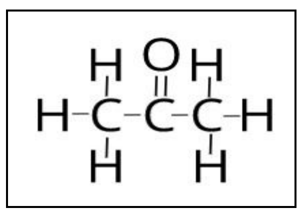


Example: The displayed structure of 3-ethyl,5-methylhexan-2-ol.

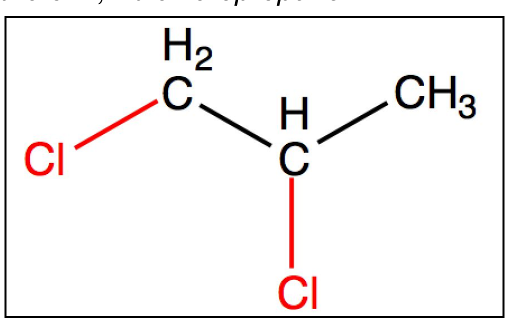


Example: The displayed structure of propanone.

Propan-2-one is also correct, but since the C=O can only be in the 2 position for the compound to be a ketone, the number is not necessary.



Example: The skeletal structure of 1,2-dichloropropane



Reaction Mechanisms

Types of reactions

Reactions can be classified according to what happens to the reactants during the reaction and what the end products are. The main types of reaction are:

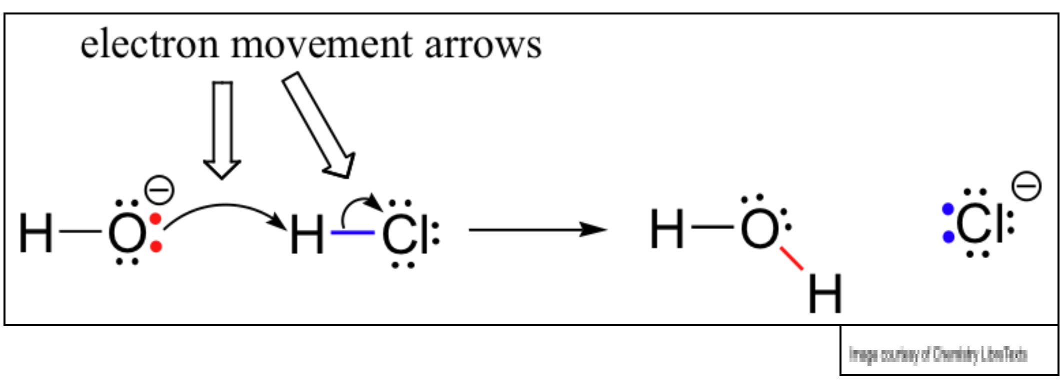
- **Addition** - In an addition reaction the reactants combine to form a **single product.**
- **Substitution** - In a substitution reaction one functional group is **replaced** by a **different functional group**.
- **Oxidation** - A species **loses** at least one electron, and is oxidised.
- **Reduction** - A species **gains** at least one electron, and is reduced.
- **Polymerisation** - A reaction in which many small molecules, known as **monomers,** join together to form a long, repeating molecule called a **polymer**.

A reaction may include **'free radicals'** or **'electrophiles'.** Free radicals are species with an **unpaired electron**, this generally makes them very **reactive**. Electrophiles are **electron acceptors** and are attracted to areas of **high electron density.**

Mechanisms

Mechanisms show the **movement of electrons** within a reaction, indicated by **curly arrows**.

Example:



Bond breaking

Reactions involve the rearrangement of atoms and bonds and therefore require breaking and making bonds. There are two types of covalent bond breaking: **homolytic** and **heterolytic**.

In **homolytic fission** the electrons in the covalent bond are divided **evenly** between the two atoms, so each atom receives one electron and forms a free radical.

In **heterolytic fission** one atom receives both electrons from the breaking of the covalent bond, while the other atom receives none. This bond-breaking forms ions. The atom that gains both of the electrons will form a negative ion and the other atom will form a positive ion.

Topic 4B: Alkanes

Introduction to Alkanes

Alkanes are **saturated hydrocarbons** where all carbon-carbon bonds are **single bonds**. Hydrocarbons are compounds containing hydrogen and carbon atoms only. They are part of a homologous series with the general formula C_nH_{2n+2}. Cycloalkanes are an exception to this general formula but are still saturated hydrocarbons.

Isomerism

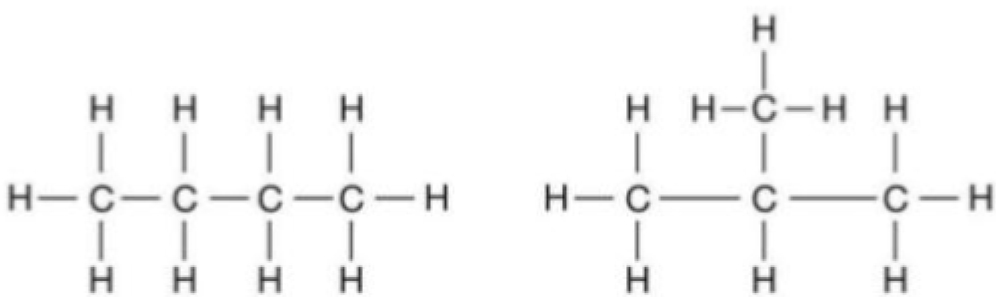
Isomers are molecules with the **same molecular formula** but a **different arrangement** of atoms within the molecule.

Structural Isomers

Structural isomers have the same molecular formula but a **different structural arrangement** of atoms. They can be **straight** chains or **branched** chains but will have the same molecular formula.

Example:

Molecular formula = C_4H_{10}



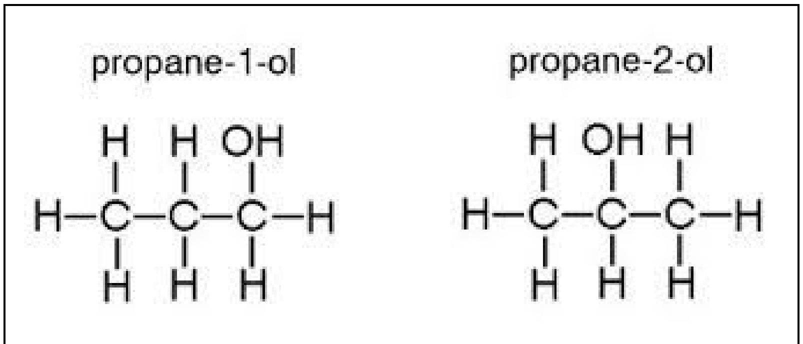
Butane 2 - methylpropane

Image courtesy of SlideShare

Position Isomers

Position isomers have the **functional group** of the molecule in a **different position** on the carbon chain.

Example:



Images courtesy of Astan Publications

Functional Group Isomers

Functional group isomers have a different arrangement of the same molecular formula so that the molecule has a **different functional group**.

Example:

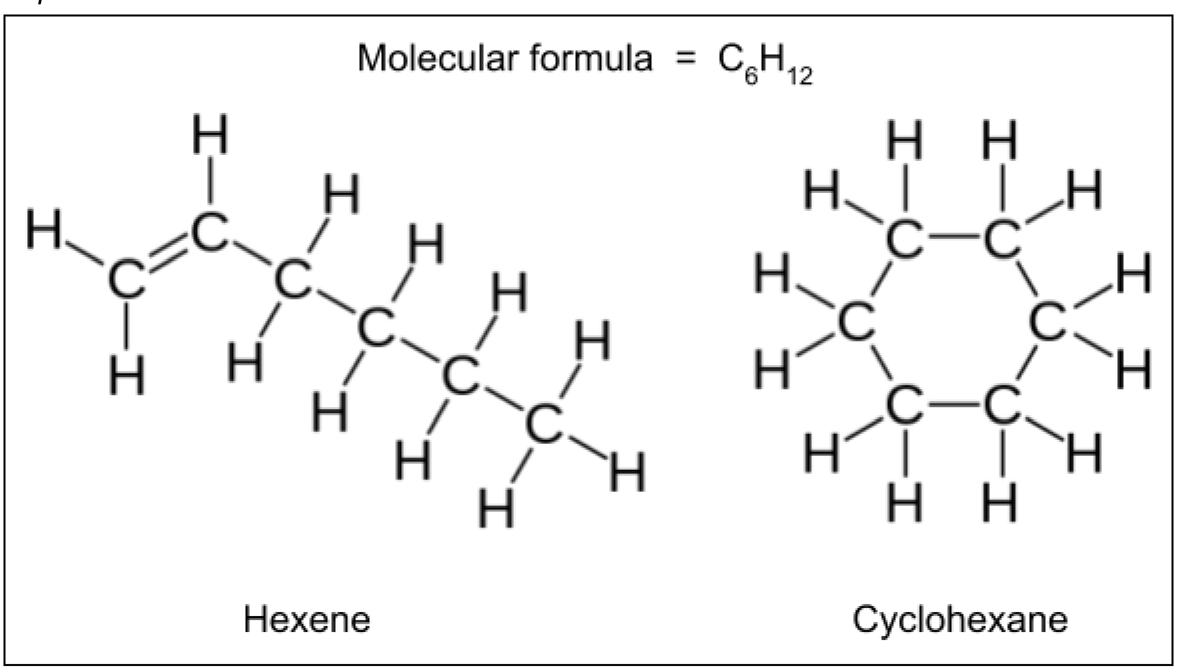


Image courtesy of Wikimedia Commons

Fractional Distillation

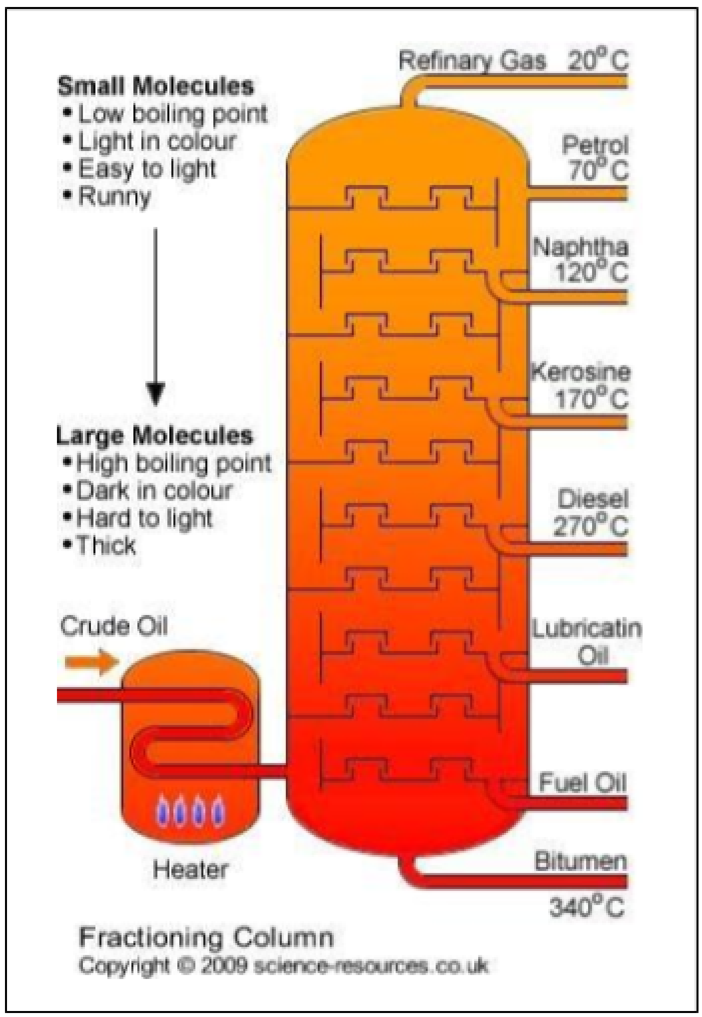
Crude oil is a mixture of different hydrocarbons. It can be separated into the separate molecules by **fractional distillation,** as the different chain lengths of molecules result in them having **different boiling points**.

Crude oil is separated in the following way:

1. The mixture is **vapourised** and fed into the fractionating column.
2. Vapours **rise, cool** and **condense**.
3. Products are **siphoned off** for different uses.

Products with **short** carbon chains have **lower** boiling points, meaning they **rise higher** up the column before reaching their boiling point. Therefore, they are **collected at the top** of the column.

Products with **long** carbon chains have **higher** boiling points, meaning they don't rise very far up the column before reaching their boiling point. They condense and are **collected at the bottom** of the fractionating column.



The compounds collected from the fractionating column are then **broken down further** via the method of **cracking**.

Cracking

Longer carbon chains are not very useful, so they are broken down to form **smaller, more useful molecules**. 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

Thermal cracking produces a high proportion of **alkanes and alkenes**. High temperatures around **1200 K** and pressures around **7000 kPa** are used to crack the carbon chains. The reaction always forms an alkane, and the remaining atoms form at least one alkene, which have the general formula C_nH_{2n}.

Examples:

$$C_{16}H_{34} \rightarrow C_{10}H_{22} + C_6H_{12}$$

$$C_{12}H_{26} \rightarrow C_4H_{10} + 4C_2H_4$$

Catalytic Cracking

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

Combustion of Alkanes

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.

Example:

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

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

Example:

$$2CH_4 + 3O_2 \longrightarrow 2CO + 4H_2O$$

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, starving the brain and other organs of oxygen and causing people to **suffocate**.

Oxides of **nitrogen** and **sulfur** are also produced as a byproduct 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:

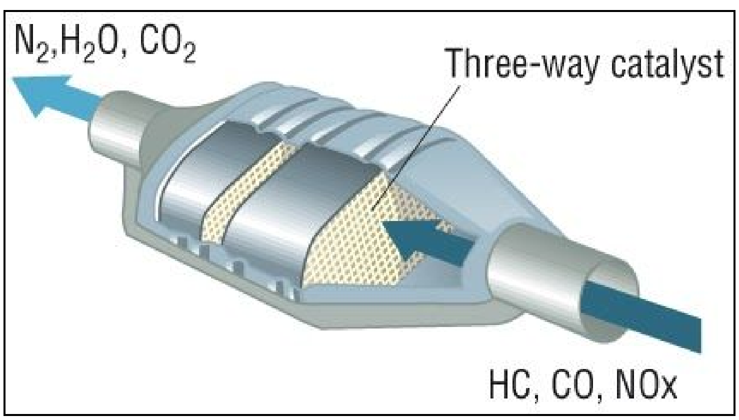


Image courtesy of thinglink.com

Alternative fuels

Alternative fuels are now being developed such as **biofuels** that release fewer, less harmful products when burned. Carbon dioxide is released during the combustion of fuels. It is a **greenhouse gas** so causes **global warming** and contributes to **climate change.**

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. It is produced by fermentation, where enzymes break down starch from crops into **sugars** which can then be **fermented to form ethanol**. It is produced in **batches**, meaning it is a relatively slow process with a **low percentage yield.** However, the environmental benefits make it viable.

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**.

Chlorination of Alkanes

Alkanes react with halogens in the presence of **UV light** to produce halogenoalkanes. The UV light breaks down the halogen bonds (homolytic fission), producing reactive intermediates called **free radicals**.

Free radicals are species containing an unpaired electron which is shown using a single dot. These attack the alkanes, resulting in a series of reactions: **initiation, propagation and termination**.

Example:

1. **Initiation** - the halogen is broken down.

$$\boxed{Cl_2 \xrightarrow{UV} 2Cl\bullet}$$

Free radicals are shown using a dot.

2. **Propagation** - a hydrogen is replaced and the Cl• radical is reformed as a catalyst.

$$Cl\bullet + CH_4 \longrightarrow \bullet CH_3 + HCl$$

$$\bullet CH_3 + Cl_2 \longrightarrow CH_3Cl + Cl\bullet$$

3. **Termination** - two radicals join to end the chain reaction and form a stable product.

$$\bullet CH_3 + \bullet CH_3 \longrightarrow C_2H_6$$

The propagation step can continue many times to result in **multiple substitutions**. This is a **chain reaction**. The condition of the reaction can be altered to favour the termination step and limit the number of substitutions, however, the nature of this reaction to produce multiple products limits its use in organic synthesis.

Mechanism

The mechanism is drawn with **half-arrows** instead of double-headed arrows. Half-arrows represent the movement of **single electrons.**