Introductory organic chemistry and alkanes

Hazard and risk, homologous series and nomenclature, isomerism, reaction types and bond fission, crude oil and its products, pollution, alternative fuels, and free-radical substitution.

Hazard and risk

A **hazard** is something that can cause harm. **Risk** is the chance that the hazard causes harm in the way it is used. A risk assessment lists the hazards in an experiment and the steps taken to reduce the risk.

Ways to reduce the risk:

- work on a **smaller scale**
- take precautions for the specific hazard (a fume cupboard for toxic gases, a water bath instead of a flame for flammable liquids, gloves and eye protection)
- use an **alternative method** with less hazardous substances

Naming organic compounds

A **homologous series** is a family of compounds with the same general formula and functional group, and with similar chemical properties. A **functional group** is the atom or group that gives a compound its characteristic reactions.

Prefixes for the length of the carbon chain:

C atoms	1	2	3	4	5	6	7	8	9	10
Prefix	meth	eth	prop	but	pent	hex	hept	oct	non	dec

IUPAC naming rules:

1. Find the **longest chain** that includes the functional group. It gives the stem.
2. Number the chain so the functional group (or the first branch) has the **lowest number**.
3. Name branches as prefixes (methyl, ethyl) in alphabetical order. Use di, tri when the same branch appears more than once, with a locant for each.
4. Write the name as one word, using commas between numbers and hyphens between numbers and letters: 2,3-dimethylbutane.

Three kinds of formula are used: **structural** (shows each carbon with its attached groups, $CH_3CH_2CH_3$), **displayed** (all atoms and bonds drawn) and **skeletal** (carbon chain as a zig-zag with hydrogens on carbons not drawn).

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Types of reaction and bond fission

Reactions are classified as **addition**, **substitution**, **oxidation**, **reduction** or **polymerisation** (and later also elimination and hydrolysis).

Bond breaking can be:

- **Homolytic** – each atom takes one electron from the bond, forming two **free radicals**. A free radical is a species with an unpaired electron, shown with a dot: $Cl\cdot$. Half-arrows (fishhooks) show the movement of one electron.
- **Heterolytic** – both electrons go to one atom, forming a cation and an anion. A full curly arrow shows the movement of an electron pair. The species formed are attacked by or attack **electrophiles** (electron-pair acceptors) or **nucleophiles**.

Alkanes

Alkanes are **saturated hydrocarbons**: they contain only carbon and hydrogen and only single bonds. The general formula is C_nH_{2n+2}; for cycloalkanes it is C_nH_{2n}.

Structural isomerism

Structural isomers have the same molecular formula but different structural formulae. They can differ in the chain (branching), the position of a functional group, or the functional group itself.

> **TRY IT**
>
> Draw and name the structural isomers of C_5H_{12}.

There are three: pentane ($CH_3CH_2CH_2CH_2CH_3$), 2-methylbutane (a methyl on carbon 2 of a four-carbon chain) and 2,2-dimethylpropane (two methyls on the central carbon of a three-carbon chain).

Crude oil and its products

Alkanes are used as fuels and are obtained from crude oil by **fractional distillation**. The crude oil is heated and the vapours rise through a column that is hotter at the bottom. Fractions condense where the temperature is below their boiling temperature. Short-chain fractions have low boiling temperatures and come off at the top; long chains stay at the bottom.

Heavy fractions are less useful, so they are converted into shorter, more valuable molecules:

- **Cracking** breaks long alkanes into shorter alkanes and alkenes, either thermally (high temperature and pressure) or catalytically with a zeolite catalyst. For example, $C_{10}H_{22} \rightarrow C_8H_{18} + C_2H_4$.
- **Reforming** converts straight-chain alkanes into branched and cyclic alkanes and arenes, which burn more smoothly and are used in petrol.

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A laboratory demonstration of cracking passes liquid paraffin vapour over hot aluminium oxide. The gaseous alkene product is collected over water and decolourises bromine water.

Combustion and pollution

Alkanes burn in plenty of air to give carbon dioxide and water:

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

In limited oxygen, **carbon monoxide** and carbon (soot) form. Other pollutants from engines are **oxides of nitrogen** (from nitrogen and oxygen in the air at high temperatures), **oxides of sulfur** (from sulfur impurities), **unburnt hydrocarbons** and **carbon particulates**.

- **Carbon monoxide** is toxic because it bonds to the iron in haemoglobin more strongly than oxygen does, so less oxygen is carried round the body.
- NO_x and SO_2 dissolve in rainwater to form acids, causing **acid rain**.

Alternative fuels

Reasons to develop alternatives: crude oil is a finite resource, and burning fossil fuels releases carbon dioxide, a greenhouse gas linked to **climate change**.

A fuel is **carbon neutral** if the carbon dioxide released on burning equals that taken in while the fuel was made. Bioethanol is close to carbon neutral, because the plants it came from absorbed carbon dioxide as they grew (although growing, harvesting and processing use energy). Petrol is not carbon neutral. **Hydrogen** produces only water on burning, but producing it can use fossil fuels or electricity.

Free-radical substitution

Alkanes are unreactive to most reagents, but they react with halogens in the presence of **ultraviolet light**.

$$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$$

The mechanism has three stages:

1. **Initiation** – UV light breaks the Cl–Cl bond homolytically: $Cl_2 \rightarrow 2Cl\cdot$
2. **Propagation** – a radical reacts to make a molecule and a new radical (a chain reaction):
   - $Cl\cdot + CH_4 \rightarrow \cdot CH_3 + HCl$
   - $\cdot CH_3 + Cl_2 \rightarrow CH_3Cl + Cl\cdot$
3. **Termination** – two radicals join and the chain stops: $Cl\cdot + Cl\cdot \rightarrow Cl_2$, $\cdot CH_3 + Cl\cdot \rightarrow CH_3Cl$, $\cdot CH_3 + \cdot CH_3 \rightarrow C_2H_6$

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The reaction is of limited use in synthesis, because further substitution gives a mixture of products (CH_2Cl_2, $CHCl_3$, CCl_4) and substitution can happen at different carbon atoms in longer chains.

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