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What do I need to know about organic chemistry?



Overview

In the nineteenth century, chemists believed that all organic chemicals originated in tissues of living organisms. Friedrich Wohler, in 1828, challenged this belief and synthesised the organic compound urea, a compound found in urine, under laboratory conditions. His work led other chemists to attempt the synthesis of other organic compounds. In this section, students examine the sources of fuels, some basic concepts of organic chemistry such as homologous series, functional group, general formula and structural formula, and polymers. Students should be able to identify and name unbranched alkanes, alkenes, alcohols and carboxylic acids. They should recognise that materials such as plastics, detergents and medicines, and even the food that we eat are examples of organic compounds. Students should be able to value the need for assessing the impacts of the use of synthetic materials and the environmental issues related to the use of plastics.

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Learning Outcomes:

Candidates should be able to:

Fuels and Crude Oil

- a) Name natural gas, mainly methane, and petroleum as sources of energy.
- b) Describe petroleum as a mixture of hydrocarbons and its separation into useful fractions by fractional distillation.
- c) Name the following fractions and state their uses:
 - i) Petrol (gasoline) as a fuel in cars.
 - ii) Naphtha as feedstock for the chemical industry.
 - iii) Paraffin (kerosene) as a fuel for heating and cooking and for aircraft engines.
 - iv) Diesel as a fuel for diesel engines.
 - v) Lubricating oils as lubricants and as a sources of polishes and waxes.
 - vi) Bitumen for making road surfaces.
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- d) State that the naphtha fraction from crude oil is the main source of hydrocarbons used as the feedstock for the production of a wide range of organic compounds.
- e) Describe the issues relating to the competing uses of oil as an energy source and as a chemical feedstock.

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Alkanes

- a) Describe an homologous series as a group of compounds with a general formula, similar chemical properties and showing a gradation in physical properties as a result of increase in the size and mass of the molecules, *e.g.* melting and boiling points; viscosity; flammability.
- b) Describe the alkanes as an homologous series of saturated hydrocarbons with the general formula C_nH_{2n+2} .
- c) Draw the structures of branched and unbranched alkanes, C1 to C4, and name the unbranched alkanes, methane to butane.
- d) Define isomerism and identify isomers.
- e) Describe the properties of alkanes (exemplified by methane) as being generally unreactive except in terms of burning and substitution by chlorine.

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Alkenes

- a) Describe the alkenes as an homologous series of unsaturated hydrocarbons with the general formula C_nH_{2n} .
- b) Draw the structures of branched and unbranched alkenes, C2 to C4, and name the unbranched alkenes, ethene to butene.
- c) Describe the manufacture of alkenes and hydrogen by cracking hydrocarbons and recognise that cracking is essential to match the demand for fractions containing smaller molecules from the refinery process.
- **d)** Describe the difference between saturated and unsaturated hydrocarbons from their molecular structures and by using aqueous bromine.
- e) Describe the properties of alkenes (exemplified by ethene) in terms of combustion, polymerisation and the addition reactions with bromine, steam and hydrogen.
- f) State the meaning of polyunsaturated when applied to food products.
- **g)** Describe the manufacture of margarine by the addition of hydrogen to unsaturated vegetable oils to form a solid product.

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Alcohols

- a) Describe the alcohols as an homologous series containing the –OH group.
- b) Draw the structures of alcohols, C1 to C4, and name the unbranched alcohols, methanol to butanol.
- c) Describe the properties of alcohols in terms of combustion and oxidation to carboxylic acids.
- d) Describe the formation of ethanol by the catalysed addition of steam to ethene and by fermentation of glucose.
- e) State some uses of ethanol, *e.g.* as a solvent; as a fuel; as a constituent of alcoholic beverages.

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Carboxylic Acids

- a) Describe the carboxylic acids as an homologous series containing the $-CO_2H$ group.
- b) Draw the structures of carboxylic acids, methanoic acid to butanoic acid and name the unbranched acids, methanoic to butanoic acids.
- c) Describe the carboxylic acids as weak acids, reacting with carbonates, bases and some metals.
- **d)** Describe the formation of ethanoic acid by the oxidation of ethanol by atmospheric oxygen or acidified potassium dichromate(VI).
- e) Describe the reaction of a carboxylic acid with an alcohol to form an ester, e.g. ethyl ethanoate.
- f) State some commercial uses of esters, *e.g.* perfumes; flavourings; solvents.

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Macromolecules

- a) Describe macromolecules as large molecules built up from small units, different macromolecules having different units and/or different linkages.
- b) Describe the formation of poly(ethene) as an example of addition polymerisation of ethene as the monomer.
- **c)** State some uses of poly(ethene) as a typical plastic, *e.g.* plastic bags; clingfilm.
- d) Deduce the structure of the polymer product from a given monomer and vice versa.
- e) Describe nylon, a polyamide, and *Terylene*, a polyester, as condensation polymers, the partial structure of nylon being represented as:



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And the partial structure of *Terylene* as:



(Details of manufacture and mechanisms of these polymerisations are not required).

- f) State some typical uses of man-made fibres such as nylon and *Terylene*,
 e.g. clothing; curtain materials; fishing line; parachutes; sleeping bags.
- **g)** Describe the pollution problems caused by the disposal of non-biodegradable plastics.

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Walk around Nanyang
 Girls' High School and take photographs of different materials that you consider to be:
 → Organic × 6.
 → Inorganic × 6.

• Upload the photographs into the shared document, clearly stating whether you consider the material to be *organic* or *inorganic*.





• The Tiger That Came to Tea – Judith Kerr – 1968



Organic Chemistry Organic Citric Acid – $C_6H_8O_7$ Ethanoic Acid – CH₃COOH Ethanol – CH_3CH_2OH $Glucose - C_6 H_{12} O_6$ Methane – CH₄ $Poly(ethene) - (CH_2CH_2)_n$ Propane – C_3H_8

Inorganic Aluminium Oxide $- Al_2O_3$ Calcium Carbonate – CaCO₃ Carbon Dioxide $- CO_2$ Copper(II) Sulfate – CuSO₄ Sodium Chloride – NaCl Sulfuric Acid – H_2SO_4 Water – H_2O

 Compare the organic compounds with the inorganic compounds. What are the differences?



• An organic compound is a compound that contains *carbon covalently bonded to hydrogen*.

Methane
 (formula CH₄)
 is organic.

H - C - H

 Carbon dioxide (formula CO₂) is *inorganic*.

O = C = O



What is the nature of the *bonding* in organic compounds?

 Because only atoms of *non-metallic elements* are present, the bonding in organic compounds is *covalent*.



Bonding in Organic Compounds Ethane $-C_2H_6$





Bonding in Organic Compounds Ethene – C_2H_4





Bonding in Organic Compounds Ethyne – C_2H_2









Bonding in Organic Compounds Ethanoic Acid – CH₃COOH





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What *properties* of carbon make it such an important element?



• Compare the bonding in the organic compounds with the bonding in the inorganic elements and compounds. What similarities and differences do you notice?



• Compare the bond strengths between i) carbon atoms, ii) carbon atoms and other elements iii) other elements (excluding carbon). What similarities and differences do you notice?

Bond	∆H kJ/mol	Bond	∆H kJ/mol	Bond	∆H kJ/mol
C – C	348	C – H	412	C = C	612
Si – Si	176	Si – H	318	$C \equiv C$	837
N - N	163	N – H	388	C – N	305
0-0	146	0 – H	463	C = N	613
P - P	172	P – H	322	$C \equiv N$	890
S – S	264	S – H	338	C – O	360
Cl - Cl	242	Cl - H	431	C - Cl	338



The Special Properties of carbon

 Carbon is in Group 14 of the Periodic Table. It has four electrons in its valence shell and therefore makes four covalent bonds with atoms of other non-metallic elements. Carbon is described as being *tetravalent*.

 The covalent bond between two carbon atoms is very strong. This allows carbon atoms to join together in large numbers to form long-chains and complex rings.
 Carbon is said to catenate.



The Special Properties of carbon



• The complex structure of the antibiotic *penicillin*.





Homologous Series

• A *homologous series* of organic compounds is a group of molecules that possess the same *functional group*, share the same *general formula* and have similar names.

 A *functional group* is a group of atoms that are bonded together in a way that is unique to that particular homologous series. The functional group is responsible for a compound's characteristic *chemical properties*.

 Because they all possess the same functional group, members of the same homologous series will all *react in* a similar way to each other.



Homologous Series – Alkanes









Homologous Series – Alkenes





• Ethene

Propene



Homologous Series – Alkenes

Functional Group



General Formula

 $C_n H_{2n}$

Name

-ene



Homologous Series – Alcohols





Ethanol

Propan-1-ol



Organic Chemistry Homologous Series – Alcohols **Functional Group** Ċ–О–Н hydroxyl $C_nH_{2n+1}OH$ **General Formula** Name -


Homologous Series – Halogenoalkanes





Bromoethane

1-Chloropropane







Homologous Series – Carboxylic Acids



нно Ч-С-С-С́ нн Ю-Н

Ethanoic Acid

Propanoic Acid



Homologous Series – Carboxylic Acids





General Formula

Name

 $C_n H_{2n} O_2$

-oic acid



Homologous Series – Esters



Ethyl Ethanoate

Methyl Propanoate







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What are the names and formulae of the *first* 10 straight chain alkanes?

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Naming Straight Chain Alkanes

• The alkanes are saturated hydrocarbons with the general formula $C_n H_{2n+2}$.

• Saturated means that the bonds between the carbon atoms are all single covalent bonds, there are no double or triple covalent bonds.

• *Hydrocarbon* means that the alkanes are composed only of the two elements *hydrogen* and *carbon*.

• General formula of $C_n H_{2n+2}$. For example, if n = 2, then $(2 \times 2) + 2 = 6$, so the formula of the alkane that contains two carbon atoms will be $C_2 H_6$.





Naming Straight Chain Alkanes

Ethane $\begin{array}{ccc} H & H \\ I & I \\ H - C - C - H \\ I & I \end{array}$ н н C_2H_6 Melting Point = -181.8°C Boiling Point = -89.0°C



Naming Straight Chain Alkanes

Propane ннн H - C - C - C - Hннн C_3H_8 Melting Point = -187.7°C Boiling Point = $-42.1^{\circ}C$



Naming Straight Chain Alkanes

Butane $\begin{array}{cccccccc} H & H & H & H \\ & & & & & \\ H - C - C - C - C - C - H \\ & & & & \\ H - H \end{array}$ нннн C_4H_{10} Melting Point = -138.4°C Boiling Point = $-0.5^{\circ}C$



Naming Straight Chain Alkanes

Pentane нннн C_5H_{12} Melting Point = $-129.8^{\circ}C$ Boiling Point = 36.1°C







Naming Straight Chain Alkanes

Heptane нннннн H - C - C - C - C - C - C - C - Hнннннн $C_7 H_{16}$ Melting Point = $-90.6^{\circ}C$ Boiling Point = 98.4°C



Organic Chemistry Naming Straight Chain Alkanes Octane нннннн H - C - C - C - C - C - C - C - C - Hннннн C_8H_{18} Melting Point = $-57.0^{\circ}C$ Boiling Point = 125.5°C



Organic Chemistry Naming Straight Chain Alkanes Nonane H H H H H H H H H нннннн $C_{9}H_{20}$ Melting Point = $-53.0^{\circ}C$ Boiling Point = 151.0°C

Naming Straight Chain Alkanes

 $C_{10}H_{22}$ Melting Point = -27.9°C Boiling Point = 174.1°C









Naming Cyclic Alkanes

Cyclobutane

H-C-C-H

-C-C-H

The prefix *cyclo*– indicates that the carbon atoms are arranged in a *ring*.

Indicates the longest carbon chain. Four carbon atoms = butane.



Physical Properties of Straight Chain Alkanes

Name	Formula	<i>M</i> _r	m.p. / °C	b.p. / °C	density / g cm ⁻³	solubility
Methane	CH ₄	16.0	-182.5	-161.6	_	The alkanes are insoluble in polar solvents such as water, but soluble in non-polar organic solvents.
Ethane	C_2H_6	30.0	-181.8	-89.0	_	
Propane	C_3H_8	44.0	-187.7	-42.1	-	
Butane	C_4H_{10}	58.0	-138.4	-0.5	_	
Pentane	C_5H_{12}	72.0	-129.8	36.1	0.626	
Hexane	C ₆ H ₁₄	86.0	-95.3	68.7	0.661	
Heptane	C ₇ H ₁₆	100.0	-90.6	98.4	0.680	
Octane	C ₈ H ₁₈	114.0	-57.0	125.5	0.703	
Nonane	C ₉ H ₂₀	128.0	-53.0	151.0	0.718	
Decane	C ₁₀ H ₂₂	142.0	-27.9	174.1	0.730	

• Viscosity (resistance to flow) *increases* as M_r and carbon chain length increase.

• Flammability *decreases* as M_r and carbon chain-length increase.

Physical Properties of Straight Chain Alkanes



- The alkanes are *non-polar* hydrocarbons. This means that their molecules do not contain any permanent regions of slight positive (δ+) or slight negative (δ–) charge.
- Alkanes are unable to form hydrogen bonds with polar water molecules.
 - As a consequence, the alkanes are immiscible (insoluble) with water.



Physical Properties of Straight Chain Alkanes

• The melting points and boiling points of the alkanes increases as the *length of the carbon chain* increases.

- The melting points and boiling points of the alkanes increases as *relative molecular mass* increases.
- A complex mixture of alkanes can be separated by fractional distillation due to differences in their boiling points.
- On an industrial scale, the complex mixture of alkanes in crude oil is separated by fractional distillation in an oil refinery.





carbon chain-length / relative molecular mass

boiling point / °C

Physical Properties of Straight Chain Alkanes



• The *melting points* and *boiling points* of the alkanes *increase* as the molecule's carbon chainlength and relative molecular mass increase.

The larger the molecule, the more electrons it contains, which increases the probability of the molecule becoming *spontaneously polarized* (regions of δ+ and δ–) due to the random movement of electrons within its larger electron cloud.



Physical Properties of Straight Chain Alkanes



• A molecule that becomes spontaneously polarized for a short time induces polarity into its neighboring molecules.

• These short-lived regions of opposite charge attract individual molecules together. These weak intermolecular forces of attraction that exist between non-polar molecules are called *London dispersion forces*.



Physical Properties of Straight Chain Alkanes



 In addition to the electron cloud, the longer an alkane's carbon chain-length, the larger its surface area. This means that there is a larger surface in contact with neighboring molecules and hence there is a larger surface area over which intermolecular forces of attraction (London dispersion forces) can operate.



Physical Properties of Straight Chain Alkanes



 A larger amount of thermal energy is required to overcome the stronger intermolecular force of attraction, hence melting points and boiling points increase as carbon chain-length and relative molecular mass increase.



Physical Properties of Straight Chain Alkanes



• As carbon chain-length increases, the liquid alkanes become *more viscous* (flows less easily).

 Molecules with longer carbon chains and higher relative molecular mass contain more electrons and become spontaneously polarized more easily. This increases the strength of the London dispersion forces between them.



Physical Properties of Straight Chain Alkanes



 In addition to the increased number of electrons, which increase the polarizability of the molecule, there is also an increase in the molecule's surface area.

 Intermolecular forces of attraction (*London dispersion forces*) become stronger, and the molecules are unable to slip-and-slide over each other as easily.



Physical Properties of Straight Chain Alkanes



• The alkanes become *less flammable* as the molecule's carbon chain-length and relative molecular mass increase.

• As the number of electrons in the molecule increases, and the surface area of the molecule increases, so the intermolecular forces of attraction (*London dispersion forces*) become stronger.



Physical Properties of Straight Chain Alkanes



• As the London dispersion forces become stronger, this causes the boiling points of the alkanes to increase, and they become less volatile, meaning that they turn from liquid to gas less readily.

 Alkanes only burn in the gaseous state. The higher the boiling point of an alkane, the less likely it is to vaporise, ignite and burn.



Physical Properties of Straight Chain Alkanes



pentane



2,2-dimethylpropane (or just dimethylpropane)

• Pentane and 2,2-dimethylpropane are *isomers*, *i.e.* they share the same molecular formula (C_5H_{12}), but have different structural formulae. Pentane boils at 31.6 $^{\circ}$ C, while 2,2-dimethylpropane boils at 9.50 °C. The difference in boiling points is due to the difference in their surface areas. The larger surface area of pentane results in stronger intermolecular forces of attraction (London dispersion forces) between the molecules, which require more energy to overcome, hence increasing the boiling point.

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How do I name the *alkenes*, *halogenoalkanes*, *alcohols* and *carboxylic acids*?



Naming Alkenes

- The alkenes are *unsaturated hydrocarbons* with the general formula $C_n H_{2n}$.
- Unsaturated means that the molecule contains at least one carbon-to-carbon double covalent bond.
 - *Hydrocarbon* means that the alkenes are composed only of the two elements *hydrogen* and *carbon*.

• General formula of $C_n H_{2n}$. For example, if n = 3, then $2 \times 3 = 6$, so the formula of the alkene that contains three carbon atoms will be $C_3 H_6$.






Naming Alkenes

Propene H H HC = C - C - HH HH C_3H_6



Naming Alkenes

But-1-ene Number: within the molecule. C_4H_8



Naming Alkenes

But-2-ene Number: $H - C = C^{1} - C^{2} = C^{3} - C^{4} - H$ Indicates the location of the C=C bond within the molecule. C_4H_8



Naming Halogenoalkanes

 The halogenoalkanes are alkanes in which at least one of the hydrogen atoms has been substituted by a halogen (Group 17 element).

 The general formula of the halogenoalkanes is *C_nH_{2n+1}Hal*, where *Hal* is the symbol of a Group 17 element (*i.e.* F, C*l*, Br, I). For example, if n = 4, then
(2 × 4) + 1 = 9, so the formula of the halogenoalkane that contains four carbon atoms and chlorine will be C₄H₉C*l*.





Naming Halogenoalkanes

Bromoethane нн H - C - C - Brн н C_2H_5Br



Naming Halogenoalkanes

Number: Indicates the location of the chlorine atom within the molecule.

1-Chloropropane $H - C^{3} - C^{2} - C^{1} - CI$ C_3H_7Cl



Naming Halogenoalkanes

2-Chloropropane $H - C_{I}^{I} - C_{I}^{2} - C_{I}^{I} - H$ Number: Indicates the location of the chlorine atom within the C_3H_7Cl molecule.



Naming Alcohols

- The alcohols are alkanes in which at least one of the hydrogen atoms has been substituted by a *hydroxyl* group, O–H.
- The general formula of the alcohols is $C_n H_{2n+1}OH$. For example, if n = 5, then $(2 \times 5) + 1 = 11$, so the formula of the alcohol that contains five carbon atoms will be $C_5H_{11}OH$.





Naming Alcohols

 $\begin{array}{c} \text{Ethanol}\\ H & H\\ H & H\\ H & H & H\\ H & H & H \end{array}$

C₂H₅OH Melting Point = -114 °C Boiling Point = 78.2 °C



Naming Alcohols

Propan-1-ol $H - C^{13} - C^{2} - C^{1} - O_{1}$ C_3H_7OH Melting Point = $-126 \circ C$ Boiling Point = 97.5 °C

Number: Indicates the location of the O–H group within the molecule.



Naming Alcohols

 $\begin{array}{c} \text{Propan-2-ol}\\ \text{H}\\ \text{H} & \text{O'H}\\ \text{H} & \text{O'H}\\ \text{H} & \text{C} & \text{C} & \text{H}\\ \text{H} & \text{H} & \text{H} \end{array}$

Number: Indicates the location of the O–H group within the molecule.

C₃H₇OH





• Hydrogen bonding between polar water molecules.





 Hydrogen bonding between the polar regions of ethanol molecules causes short-chain alcohols to be liquids at room temperature and pressure (recall that short chain alkanes and alkenes of a similar relative molecular mass are gases).

Physical Properties of Alcohols





Physical Properties of Alcohols



 The polar hydrophilic region of ethanol is more significant than the small non-polar hydrophobic region, and dominates the properties of the molecule, causing it to be miscible (soluble) with water (ethanol is infinitely soluble in water).

Physical Properties of Alcohols







• The large non-polar *hydrophobic* region of hexan-1-ol is more significant than the polar *hydrophilic* region, and dominates the properties of the molecule, causing it to be *immiscible* (insoluble) with water.



Physical Properties of Alcohols

Name	Formula	Melting point / °C	Boiling point / °C	*Solubility in water
methanol	CH₃OH	-97.6	64.7	miscible / ∞ soluble
ethanol	C_2H_5OH	-114	78.2	miscible / ∞ soluble
propan-1-ol	C ₃ H ₇ OH	-126	97.5	miscible / ∞ soluble
butan-1-ol	C₄H ₉ OH	-89.8	117.7	73
pentan-1-ol	C ₅ H ₁₁ OH	-78	137	22
hexan-1-ol	C ₆ H ₁₃ OH	-45	157	5.9

*Solubility measured in grams of alcohol per 1000 cm³ of water at 20°C.

• The first six straight-chain alcohols are *colourless liquids* at room temp. and pressure.

• Melting points and boiling points *increase* as carbon chain-length *increases*.

• Solubility in water *decreases* as carbon chain-length *increases*.

Naming Carboxylic Acids

• The general formula of the carboxylic acids is $C_n H_{2n} O_2$. For example, if n = 6, then 2 × 6 = 12, so the formula of the carboxylic acid that contains six carbon atoms will be $C_6 H_{12} O_2$.

Note: The carboxylic acid functional group is COOH (*carboxyl*). This is normally written separately in the formula, so $C_6H_{12}O_2$ is re-written as $C_5H_{11}COOH$.

 Remember, the carboxylic acids are weak acids, i.e. they only partially ionise when dissolved in water.

 $CH_3COOH \rightleftharpoons CH_3COO^- + H^+$







Naming Carboxylic Acids

Ethanoic Acid



CH₃COOH



Naming Carboxylic Acids

Propanoic Acid $\begin{array}{cccc} H & H & O \\ I & I & \gamma' \\ H - C - C - C \\ I & I & 0 - H \\ H & H & 0 - H \end{array}$ C₂H₅COOH



Naming Carboxylic Acids

Butanoic Acid

 C_3H_7COOH



Organic Chemistry Physical Properties of Carboxylic Acids -δ+ δ+ $\delta +$

• Hydrogen bonding between polar water molecules.



Physical Properties of Carboxylic Acids



polar regions of ethanoic acid molecules causes ethanoic acid to be a *liquid* at room temperature and pressure.



Physical Properties of Carboxylic Acids





Physical Properties of Carboxylic Acids



 The polar *hydrophilic* region of ethanoic acid is more significant than the small non-polar *hydrophobic* region, and dominates the properties of the molecule, causing it to be *miscible* (soluble) with water (ethanoic acid is infinitely soluble in water).

Physical Properties of Carboxylic Acids







 The larger, non-polar, *hydrophobic* region of hexanoic acid is more significant than the polar *hydrophilic* region, and dominates the properties of the molecule, causing it to be *immiscible* (insoluble) with water.

Physical Properties of Carboxylic Acids

Name	Formula	Melting point / °C	Boiling point / °C	*Solubility in water
methanoic acid	нсоон	8.4	101	miscible / ∞ soluble
ethanoic acid	CH ₃ COOH	16.5	118.5	miscible / ∞ soluble
propanoic acid	C ₂ H ₅ COOH	-20.5	141	miscible / ∞ soluble
butanoic acid	C ₃ H ₇ COOH	-5.1	163.8	miscible / ∞ soluble
pentanoic acid	C ₄ H ₉ COOH	-34.5	185	49.7
hexanoic acid	C ₅ H ₁₁ COOH	-3.4	205.8	10.8

*Solubility measured in grams of carboxylic acid per 1000 cm³ of water at 20°C.

• The first six carboxylic acids are *colourless liquids* at room temperature and pressure.

• Boiling points *increase* as carbon chain-length *increases*.

• Solubility in water *decreases* as carbon chain-length *increases*.



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How do I name organic compounds that have *more than one functional group*?



Hierarchy of Functional Groups in Naming Compounds

 Chemical nomenclature is a set of rules used to generate systematic names for chemical compounds. The nomenclature used most frequently worldwide is the one created and developed by the International Union of Pure and Applied Chemistry (IUPAC).

 Ideally, every possible organic compound should have a name from which an unambiguous structural formula can be created. IUPAC Nomenclature ensures that each organic compound (and its various isomers) has only one formally accepted name known as the systematic IUPAC name.



Hierarchy of Functional Groups in Naming Compounds



assigned to them when naming.


Hierarchy of Functional Groups in Naming Compounds





Hierarchy of Functional Groups in Naming Compounds



1,1-dibromo-1-chloroethane

• Longest carbon chain = 2, hence the name <u>ethane</u>.

• Bromo- and chloro- are arranged in alphabetical order.

• Di- means '2', hence dibromo means '2 atoms of bromine' (tri- means '3').

• Numbers are used to identify the locations of –Br and –Cl

in the molecule to avoid any ambiguity.



Hierarchy of Functional Groups in Naming Compounds





Hierarchy of Functional Groups in Naming Compounds



3-methylbutan-2-ol (not 2-methylbutan-3-ol)

• Longest carbon chain = 4, hence the name *butanol*.

• The hydroxyl group takes priority and is assigned the smallest number.

 Numbers are used to identify the locations of –CH₃ and –OH in the molecule to avoid any ambiguity.



Hierarchy of Functional Groups in Naming Compounds





Hierarchy of Functional Groups in Naming Compounds



5-bromo-3-methylpent-1-ene

- The longest carbon chain = 5, hence the name *pentene*.
- The alkene group takes priority and is assigned the smallest number.
 - Bromo- and methyl- are arranged in alphabetical order.
 - Numbers are used to identify the locations of –Br, –CH₃ and C=C in the molecule to avoid any ambiguity.



Hierarchy of Functional Groups in Naming Compounds





Hierarchy of Functional Groups in Naming Compounds



Hex-4-en-1-ol (*not* hex-2-en-6-ol)

The longest carbon chain = 6, hence the name <u>hexenol</u>.
The hydroxyl group takes priority and is assigned the smallest number.
Numbers are used to identify the locations of C=C and –OH in the molecule to avoid any ambiguity.



Hierarchy of Functional Groups in Naming Compounds





Hierarchy of Functional Groups in Naming Compounds



3-bromo-4-chloro-2,2-dimethylbutanoic acid

- The longest carbon chain = 4, hence the name *butanoic acid*.
- The carboxylic acid group takes priority and is assigned the value of 1.
 - Bromo-, chloro- and methyl are arranged in alphabetical order.
- Di- means '2', hence dimethyl means '2 methyl groups' (tri- means '3').
 - Numbers are used to identify the locations of -Br, -Cl and $-CH_3$ in the molecule to avoid any ambiguity.



Hierarchy of Functional Groups in Naming Compounds





Hierarchy of Functional Groups in Naming Compounds



5-bromo-4-methylpent-2-en-1-ol

The longest carbon chain = 5, hence the name <u>pentenol</u>.
The hydroxyl group takes priority and is assigned the smallest number.
Bromo- and methyl- are arranged in alphabetical order.
Numbers are used to identify the locations of -Br, -CH₃, C=C and -OH in the molecule to avoid any ambiguity.



What is the origin of the organic compounds that are used by chemists?





Origin of Crude Oil (Petroleum)

 Millions of years ago, prehistoric plankton and algae died and sank to the seabed. Over time, the dead organisms were slowly covered by layers of silt and sand.

 Heat from the Earth and pressure from the silt and sand acted on these organisms over millions of years. In the absence of oxygen (anaerobic conditions), complex organic compounds in the organisms transformed into crude oil (petroleum) and natural gas.

 Petroleum and natural gas are often found in underground deposits hundreds, or thousands, of metres below the surface of the Earth. Deep wells must be drilled to extract them.

Origin of Crude Oil (Petroleum)



Origin of Crude Oil (Petroleum)

- Crude oil (petroleum) is a very complex mixture of organic compounds.
- Crude oil is a dark brown, toxic, foul smelling and viscous liquid.
- Crude oil can be separated into useful fractions by fractional distillation in an oil refinery.

 Each crude oil fraction is a mixture of hydrocarbons that boils over a certain range of temperatures.
 → Lighter fractions (low b.p.) consist of smaller hydrocarbons.
 → Heavier fractions (high b.p.) consist of larger hydrocarbons.

Fractional Distillation of Crude Oil (Petroleum)



• Diagram to illustrate some uses of the different fractions that are separated from crude oil.



Fractional Distillation of Crude Oil (Petroleum)



• Petrol – C_5H_{12} to $C_{10}H_{22}$ – is an important fraction that is separated from crude oil by *fractional distillation*.



Fractional Distillation of Crude Oil (Petroleum)



Fractional Distillation of Crude Oil (Petroleum)

Name of Fraction	Number of Carbon Atoms	Boiling Point / °C	Use of Fraction
Petroleum Gas	$C_{1} - C_{4}$	< 40	Fuel for cooking and heating.
Petrol (Gasoline)	$C_{5} - C_{10}$	40 – 75	Fuel for motorcars.
Naphtha	$C_7 - C_{14}$	90 – 150	Feedstock for the chemical industry.
Paraffin (Kerosene)	$C_9 - C_{16}$	150 – 240	Fuel for aircraft, cooking and heating.
Diesel Oil	$C_{15} - C_{25}$	220 – 250	Fuel for buses, lorries and trains.
Lubricating Oil	$C_{20} - C_{35}$	300 – 350	For lubricating machines.
Bitumen	> C ₇₀	> 350	For making road surfaces and roofing.



Fractional Distillation of Crude Oil (Petroleum)

• A single barrel of crude oil – once it has been refined – can yield a large number of different, useful petroleum products. The refining process separates these different hydrocarbons by virtue of their different boiling points in a fractional distillation tower. Note that a very large proportion of the crude oil is used as fuel, and only a relatively small proportion is used for manufacturing.





https://energyeducation.ca/encyclopedia/in_a_barrel_of_oil

Fractional Distillation of Crude Oil (Petroleum)

 As the relative molecular mass of the hydrocarbons in a fraction increases, so the colour of the fractions gradually become darker.



 This is because, as the relative molecular masses of the molecules in the fractions increases, so the bonding within the molecules becomes more complex, *e.g.* -CH=CH–CH=CH–. Electrons within these molecules are able to absorb light in the visible spectrum, and hence the fractions become coloured.

Fractional Distillation of Crude Oil (Petroleum)

• As the relative molecular mass of the hydrocarbons in a fraction increases, so the colour of the fractions gradually become darker.



Low Relative Molecular Mass

- Short carbon chains
 - Low melting point
 - Low boiling point
 - Low viscosity
 - High flammability
 - Pale colour

High Relative Molecular Mass

- Long carbon chains
 - High melting point
 - High boiling point
 - High viscosity
 - Low flammability
 - Dark colour



Fractional Distillation of Crude Oil (Petroleum)

The catalytic cracking of long-chain alkanes produces shortchain alkanes and alkenes as reaction products. Short-chain alkanes tend to be more useful than long-chain alkanes, and alkenes can be used in organic synthesis.





Fractional Distillation of Crude Oil (Petroleum)

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Fractional Distillation of Crude Oil (Petroleum)

The catalytic cracking of long-chain alkanes produces shortchain alkanes and alkenes as reaction products. Short-chain alkanes tend to be more useful than long-chain alkanes, and alkenes can be used in organic synthesis.



Fractional Distillation of Crude Oil (Petroleum)



 An experiment to crack a long-chain hydrocarbon in the lab. Note that the insoluble ethene gas is collected by the downward displacement of water.



Fractional Distillation of Crude Oil (Petroleum)



Fractional Distillation of Crude Oil (Petroleum)

- Accidents during the transport of crude oil can lead to environmental disasters.
- The non-polar hydrocarbon molecules in crude oil are immiscible with the polar solvent water.
 - Crude oil is less dense than water.

 The crude oil coats plants and animals with a thick, viscous layer of toxic chemicals which will eventually kill them if not removed.



Fractional Distillation of Crude Oil (Petroleum)



Fractional Distillation of Crude Oil (Petroleum)

 Crude oil, coal and natural gas are fossil fuels.
 They are non-renewable sources of energy, and will eventually run out.

 It is important to develop alternative sources of clean and renewable energy.



Fractional Distillation of Crude Oil (Petroleum)



Fractional Distillation of Crude Oil (Petroleum)

- The combustion of fossil fuels produce pollutants such as:
- Carbon dioxide \rightarrow causes global warming.

• Carbon monoxide \rightarrow toxic.

- Oxides of nitrogen \rightarrow irritant, causes acid rain.
 - Sulfur dioxide \rightarrow irritant, causes acid rain.
 - Unburned hydrocarbons \rightarrow cause cancer.



Fractional Distillation of Crude Oil (Petroleum)



 Pollutants can be removed from car exhaust fumes using *catalytic converters*. For example: 2CO(g) + 2NO(g) → 2CO₂(g) + N₂(g)


Structural Isomerism

- Structural isomers are compounds that share the same molecular formula, but have different structural formulas (arrangement of atoms).
 - Isomers may or may not belong to the same homologous series.
 - Isomers have different names.



There are Two Isomers of C_4H_{10} :







2-methylpropane (or just methylpropane)



This is butane *not* 1-methylpropane





This is butane *not* 1-methylpropane



This is butane *not* 1,2-dimethylethane

• Take care when drawing the structural formulae of organic compounds.



 What is wrong with the structural formulae of these three organic compounds?



 Take care when drawing the structural formulae of organic compounds.





Carbon making 3 bonds instead of 4 bonds.

Hydrogen making 2 bonds instead of only 1 bond.

Carbon making 5 bonds instead of only 4 bonds.

 What is wrong with the structural formulae of these three organic compounds?



What are the Isomers of C_4H_9Br ?



What are the Isomers of C₄H₉Br?



1-bromobutane



1-bromo-2-methylpropane (or just 1-bromomethylpropane)



2-bromobutane



2-bromo-2-methylpropane (or just 2-bromomethylpropane)



What are the Isomers of C_5H_{12} ?



What are the Isomers of C_5H_{12} ?





H C I H C I H C H H C H H C H

pentane

2-methylbutane (or just methylbutane)

2,2-dimethylpropane (or just dimethylpropane)



What are the Isomers of C_6H_{14} ?



What are the Isomers of C_6H_{14} ?







hexane

2-methylpentane

3-methylpentane



2,2-dimethylbutane



2,3-dimethylbutane



What are the Isomers of C_4H_8 ?

What are the Isomers of C_4H_8 ?



Structural Isomerism

• As the number of carbon atoms and hydrogen atoms in an alkane gradually increases, so the number of structural isomers increases very rapidly.

 \rightarrow Octane, C₈H₁₈, has **18** isomers

 \rightarrow Decane, C₁₀H₂₂, has **75** isomers

 \rightarrow Dodecane, C₁₂H₂₆, has 355 isomers



How do I *calculate the formula* of an organic compound from its percentage composition?



Calculation of Formula from Percentage Composition

 Calculate the empirical formula of the hydrocarbon that has the following percentage composition:

C = 85.7% H = 14.3 %

 Given that the relative molecular mass of the hydrocarbon is 42.0, calculate the molecular formula of the hydrocarbon.

• This hydrocarbon has two isomers. Give the structural formulae and names of the two isomers.



Calculation of Formula from Percentage Composition

Step 1: Divide each element's percentage by the element's relative atomic mass.

• For carbon: 85.7 ÷ 12.0 = 7.14

• For hydrogen: 14.3 ÷ 1.0 = 14.3

How does this calculation work? Imagine that you had 100 g of the hydrocarbon. 85.7 g of the compound would be carbon, and 14.3 g would be hydrogen. Remember, mass in grams divided by relative atomic mass gives number of moles as the answer. So, 85.7 ÷ 12.0 = 7.14 moles of carbon and 14.3 ÷ 1.0 = 14.3 moles of hydrogen. The simple mole ratio of elements in a compound gives us the empirical formula of the compound.



Calculation of Formula from Percentage Composition

Step 2: Divide each one of the answers by the smallest answer.

- For carbon: 7.14 ÷ 7.14 = 1.00
- For hydrogen: 14.3 ÷ 7.14 = 2.00



Calculation of Formula from Percentage Composition

Step 3: This gives the compound's empirical formula which is the most simple ratio of elements in the compound.

 CH_2



Calculation of Formula from Percentage Composition

Step 4: Calculate the relative molecular mass of the compound's empirical formula.

 $= C + (2 \times H)$ = 12.0 + (2 × 1.0) = 14.0



Calculation of Formula from Percentage Composition

Step 5: Divide the relative molecular mass of the compound's molecular formula by the relative molecular mass of the compound's empirical formula.

 $= 42.0 \div 14.0$

= 3.00



Calculation of Formula from Percentage Composition

Step 6: Multiply the empirical formula by the answer to Step 5 to determine the compound's molecular formula.

 $= CH_2 \times 3.00$

 C_3H_6



Calculation of Formula from Percentage Composition





Propene

Cyclopropane



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

 The complete combustion of a hydrocarbon will produce carbon dioxide gas and water – in the form of steam – as the reaction products.

$$C_{x}H_{y} + \left(x + \frac{y}{4}\right)O_{2} \rightarrow xCO_{2} + \frac{y}{2}H_{2}O_{2}$$



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

• Remember, the formula of a compound is an expression of how many moles of each constituent element are present in one mole of the compound.

The number of moles of hydrocarbon X, moles of hydrogen and moles of carbon can each be determined from the volumes of gases that are given in the question: moles of gas = volume of gas in cm³ ÷ 24 000
 Recall: 1 mol of gas occupies 24 000 cm³ at room temperature & pressure.



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

 a) Calculate moles of gaseous hydrocarbon X that were burned:

= volume of hydrocarbon **X** in $cm^3 \div 24\ 000$

= 20 ÷ 24 000

= 0.0008333 mol



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

- On cooling, the volume of gaseous product decreased by 100 cm³ because the steam condensed.
 - b) Calculate moles of steam H₂O(g) that were produced:
 - = volume of steam in $cm^3 \div 24\ 000$
 - = 100 ÷ 24 000
 - = 0.004167 mol of steam



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

 1 mol of steam – H₂O(g) – contains 2 mol of hydrogen atoms – H.

 c) Calculate moles of hydrogen atoms present in 0.0008333 mol of hydrocarbon X:

= 0.004167 × 2

= 0.008334 mol of hydrogen atoms



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

 d) Calculate moles of hydrogen atoms present in 1 mol of hydrocarbon X:

0.0008333 mol of hydrocarbon **X** contains 0.008334 mol of hydrogen atoms

 $\therefore 0.0008333 \div 0.0008333$ mol of hydrocarbon \boldsymbol{X} contains $0.008334 \div 0.0008333$ mol of hydrogen atoms

∴ 1 mol of hydrocarbon X contains 10.0 mol of hydrogen atoms



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

• The volume decreased by 80 cm³ because carbon dioxide (acid) was absorbed by sodium hydroxide (alkali).

- e) Calculate moles of carbon dioxide CO₂(g) that were produced:
 - = volume of carbon dioxide in $cm^3 \div 24000$

= 80 ÷ 24 000

= 0.003333 mol of carbon dioxide



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

 1 mol of carbon dioxide – CO₂(g) – contains 1 mol of carbon atoms – C.

 f) Calculate moles of carbon atoms present in 0.0008333 mol of hydrocarbon X:

= 0.003333 × 1

= 0.003333 mol of carbon atoms



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

g) Calculate moles of carbon atoms present in
1 mol of hydrocarbon X:

0.0008333 mol of hydrocarbon **X** contains 0.003333 mol of carbon atoms

 $\therefore 0.0008333 \div 0.0008333$ mol of hydrocarbon \boldsymbol{X} contains $0.003333 \div 0.0008333$ mol of carbon atoms

∴ 1 mol of hydrocarbon X contains 4.00 mol of carbon atoms



Question: 20 cm³ of gaseous hydrocarbon X was completely burned in oxygen. On cooling, the gaseous product contracted in volume by 100 cm³. After bubbling through concentrated aqueous sodium hydroxide, the volume contracted again by another 80 cm³. Calculate the molecular formula of hydrocarbon X.

h) State the molecular formula of hydrocarbon X:

- 1 mol of hydrocarbon X contains 4 mol of carbon atoms.
- 1 mol of hydrocarbon **X** contains 10 mol of hydrogen atoms.
- The molecular formula of hydrocarbon **X** is C_4H_{10} .





Presentation on Organic Chemistry by Dr. Chris Slatter

christopher_john_slatter@nygh.edu.sg

Nanyang Girls' High School 2 Linden Drive Singapore 288683

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