## Hydrocarbons

**Inquiry question:** How can hydrocarbons be classified based on their structure and reactivity?

Students:

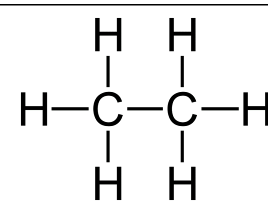
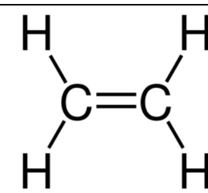
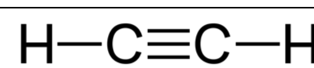
- construct models, identify the functional group, and write structural and molecular formulae for homologous series of organic chemical compounds, up to C8 (ACSCH035):
  - alkanes
  - alkenes
  - alkynes
- conduct an investigation to compare the properties of organic chemical compounds within a homologous series, and explain these differences in terms of bonding (ACSCH035)
- analyse the shape of molecules formed between carbon atoms when a single, double or triple bond is formed between them
- explain the properties within and between the homologous series of alkanes with reference to the intermolecular and intramolecular bonding present
- describe the procedures required to safely handle and dispose of organic substances (ACSCH075)
- examine the environmental, economic and sociocultural implications of obtaining and using hydrocarbons from the Earth
- explore and distinguish the different types of structural isomers, including saturated and unsaturated hydrocarbons, including: (ACSCH035)
  - chain isomers
  - position isomers
  - functional group isomers

## Introduction to Organic Chemistry

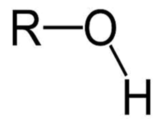
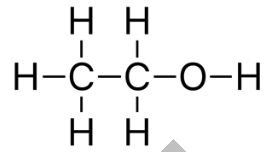
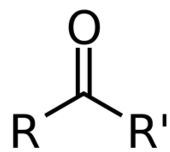
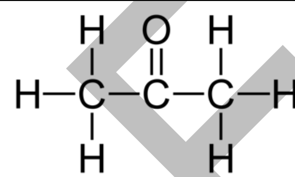
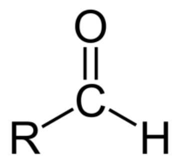
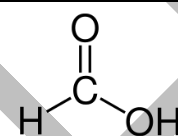
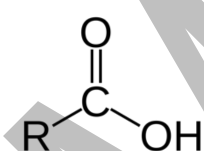
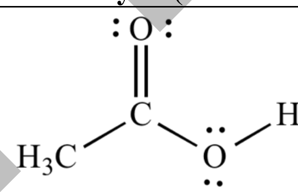
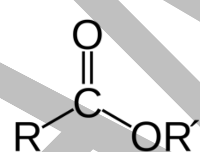
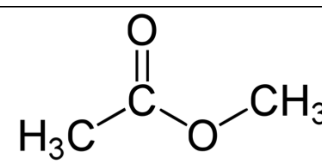
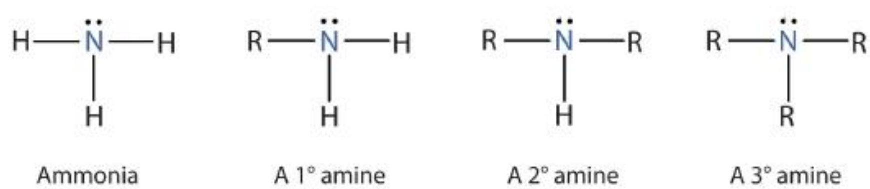
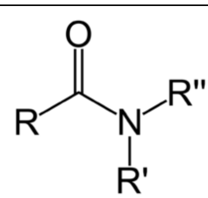
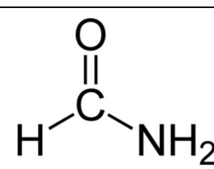
- Organic chemistry involves reactions of carbon-based compounds. All compounds which contain carbon are considered organic except:
  - Oxides of carbon e.g. carbon dioxide, carbon monoxide.
  - Compounds consisting of carbon but form ionic compounds e.g. cyanide ($CN^-$).

- Carbon is the building block of life because it can bond with up to 4 atoms. This allows for the creation of a diverse range of molecules.
  - Protein (polypeptide)
  - Deoxyribonucleic acid (DNA)
  - Sugar (e.g. glucose, sucrose)
  - Fats (fatty acids)

**Hydrocarbons**
- Hydrocarbons are organic compounds that consist of carbon and hydrogen atoms only.
- Carbon to carbon and C–H bonds are strong and unreactive. These bonds provide hydrocarbons with solid scaffolds.
- Hydrocarbons can have three functional groups or homologous series.
- **Functional group:** a group of atoms that provides a particular characteristic or is responsible for a reaction of a compound.
- **Homologous series:** a series of compounds with the same functional group and similar chemical properties.

| *Homologous series* | *Distinguishing feature* | *General molecular formula* | *Example* |
|---|---|---|---|
| Alkane | C–C | $C_nH_{2n+2}$ |  ethane |
| Alkene | C=C bond(s) | $C_nH_{2n}$ |  ethene |
| Alkyne | C≡C bond(s) | $C_nH_{2n-2}$ |  ethyne |

**An overview of other common functional groups**

| *Functional group* | *Generic structure* | *Example* |
|---|---|---|
| Alcohol |  |  ethan**ol** |
| Ketone |  |  propan**one** |
| Aldehyde |  |  methan**aldehyde** (formaldehyde) |
| Carboxylic acid |  |  ethan**oic acid** |
| Ester |  |  methyl ethan**oate** |
| Amine |   | |
| Amide |  |  methan**amide** (formamide) |

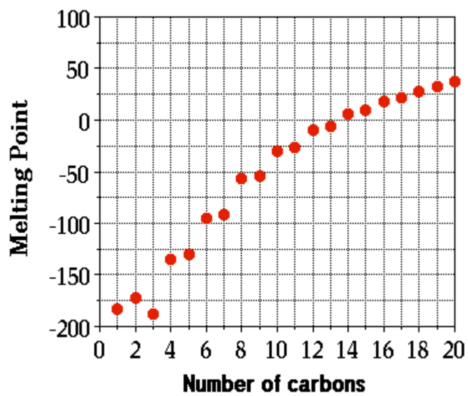
**Alkanes**

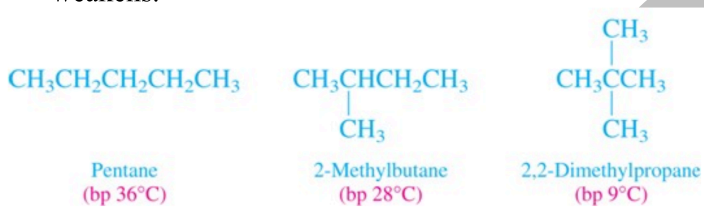
- Alkanes are typically used as fuel e.g. natural gas and fossil fuel to produce large amounts of energy. Smaller, short-chained alkanes combust more efficiently than larger alkanes. For example, the complete combustion of propane ($C_3H_8$) yield carbon dioxide and water.

$$2C_3H_{8(g)} + 7O_{2(g)} \rightarrow 6CO_{2(g)} + 8H_2O_{(g)}$$

- Alkanes are non-polar hydrocarbons held together by dispersion forces as its main intermolecular force. Thus, the molecular weight or size of alkanes largely determines the strength of dispersion force and physical properties such as melting and boiling points.

- Branched alkanes typically have lower melting and boiling points because the presence of substituents forces carbon chains to become further away from each other. As a result, intermolecular forces i.e. dispersion force weakens.



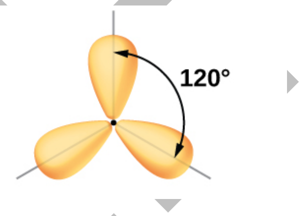
**Alkene**

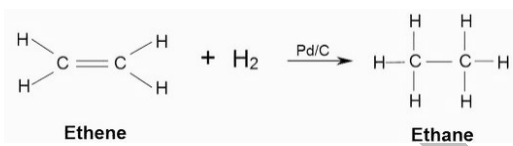
- The melting and boiling points of hydrocarbons in the alkene homologous series behave in the same way as alkenes. As the number of carbon atoms and the molecular weight of alkenes increase, the strength of dispersion forces increases. As a result, melting point and boiling point increase with size.

- Since alkene molecules have two less electrons than an alkane of the same number of carbons, its dispersion force is slightly weaker. Consequently, the melting and boiling point of alkenes are a few degrees lower than those of alkanes.

- **Alkenes are more reactive than alkanes** due to the presence of an electron-dense double bond (π-bond). The electrons in the double bond can easily react with other molecules by forming a new bond.

- When a carbon atom is connected to another carbon atom via a C=C double bond, it is connected to a total of 3 atoms. This means it exists in a trigonal planar shape with each bond subtended at a 120º angle relative to one another.

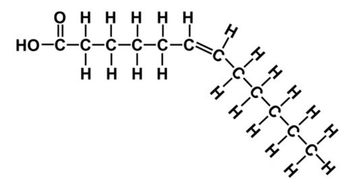


Ethene
Ethane

- Alkenes are unsaturated hydrocarbons because the double bond(s) can further react to add more hydrogen atoms. This process of transforming an alkene into an alkane is called hydrogenation.

Unsaturated Fatty Acid

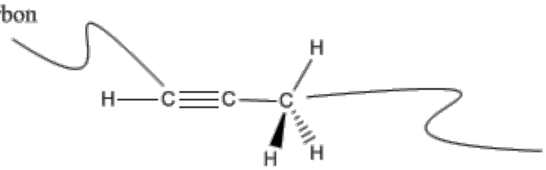


**Alkynes**

- Alkynes have higher melting and boiling point than both alkanes and alkenes with the same number of carbon atoms, despite having less electrons. There are a few more factors that contribute to intermolecular force in alkynes:
  - The electrons in the triple bond are more easily polarised to create induced dipole-dipole forces which increases the overall attraction between alkyne molecules
  - Alkynes have less C–H bonds which means alkyne molecules can move closer together, further increasing the strength of their intermolecular forces.

- Alkynes are more reactive than alkenes and alkanes.

- Carbon atoms in a triple carbon-to-carbon bond are only connected to two atoms. As a result, they exist in a linear shape with each bond subtended at 180º angle relative to one another. In other words, the σ-bond (C–H) lies in the same plane as the π-bonds.

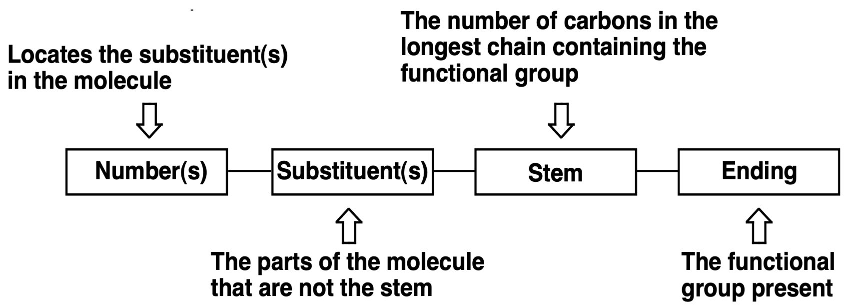


propyne

- Similar to alkenes, alkynes are unsaturated hydrocarbons

## Naming Hydrocarbons (Nomenclature)

- Nomenclature of organic carbons including hydrocarbons must account for:
  - Functional group(s) and their positions
  - Number of carbon atoms in the longest chain (stem)
  - Type and position of substituents



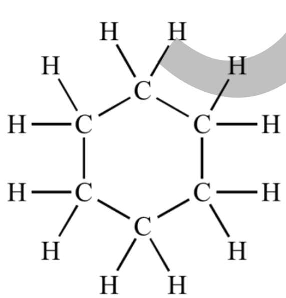

**Number of carbon atoms in the longest chain**

| *No. of Carbons* | *Name* | *Molecular formula* |
|---|---|---|
| 1 | **Meth**ane | $CH_4$ |
| 2 | **Eth**ane | $C_2H_6$ |
| 3 | **Prop**ane | $C_3H_8$ |
| 4 | **But**ane | $C_4H_{10}$ |
| 5 | **Pent**ane | $C_5H_{12}$ |
| 6 | **Hex**ane | $C_6H_{14}$ |
| 7 | **Hept**ane | $C_7H_{16}$ |
| 8 | **Oct**ane | $C_8H_{18}$ |

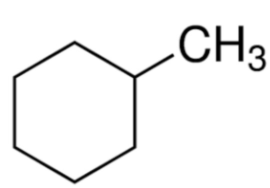
**Function group of hydrocarbons**

| *Functional group* | *Suffix* | *Example* |
|---|---|---|
| Alkane | -ane | Eth**ane** |
| Alkene | -ene | Eth**ene** |
| Alkyne | -yne | Eth**yne** |

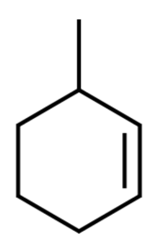
- Alkanes and alkenes can have cyclo- compounds in which the longest carbon chain forms a ring. This unique type of hydrocarbon is specified by a prefix of 'cyclo' before its functional group part.


Cyclohexane


Cyclopentene

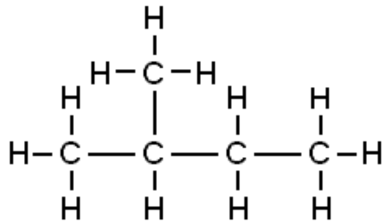
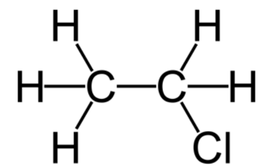
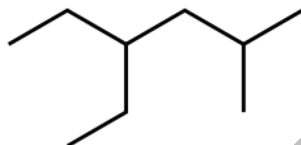
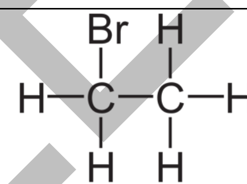
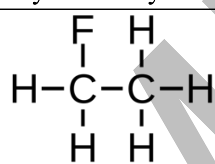
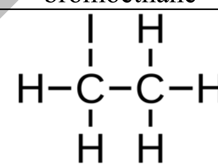


Methylcyclohexane


3-methylcyclohexene

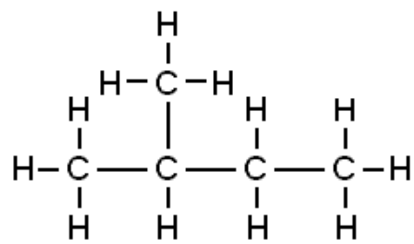
**Common Substituents for Hydrocarbons**

- In addition to the longest carbon chain, hydrocarbons can have ‘branches’ or formally – substituents. Substituents are denoted in the name as a prefix.

| *Substituent* | *Prefix* | *Example* | *Substituent* | *Prefix* | *Example* |
|---|---|---|---|---|---|
| $–CH_3$ | Methyl- |  2-Methylbutane | –Cl | Chloro- |  chloroethane |
| $–CH_2CH_3$ | Ethyl- |  3-ethyl-2-methylhexane | –Br | Bromo- |  bromoethane |
| –F | Fluoro- |  Fluoroethane | –I | Iodo- |  iodoethane |

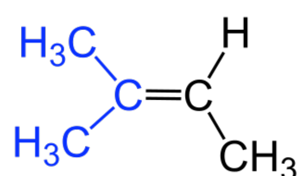
**IUPAC Rules for naming**

1. Find the longest continuous carbon chain containing the principal functional group. This will help identify which carbons belong to a substituent group.



2-methylbutane

2. Number the carbon chain such that the functional group receives the smallest number. After prioritising the functional group, the substituents should also receive the smallest number possible.



2-methyl-but-2-ene or 2-methyl-2-butene

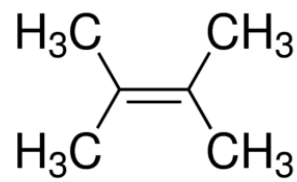
3. Name each substituent and indicate the position (separate by a '–')

4. If two or more identical substituent groups are present, specify using the prefix:

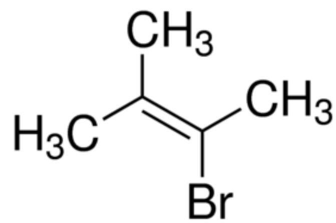
5.

| | |
|---|---|
| di | Two identical groups |
| tri | Three identical groups |
| tetra | Four identical groups |

6. If there are more than one substituent, arrange them in alphabetical order. If the sum of their positions remains the same, the first substituent (after rearrangement) should have the smaller number.



2,3-dimethyl-2-butene



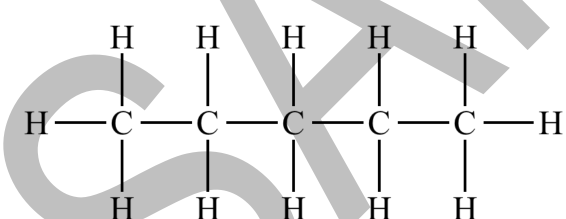
2-bromo-3-methyl-2-butene

## Isomers

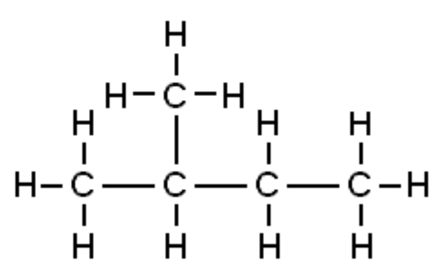
- Isomers are compounds which share the same molecular formula but different structure. There are three types of isomers to be explored in HSC Chemistry.

**Chain isomers**

- Chain isomers are molecules with the same molecular formula, but different arrangement of its carbon chain (stem).
- For example, pentane and 2-methyl butane are both alkanes with five carbon atoms and therefore the same molecular formula $C_5H_{12}$. Yet, they are different structural formulae.



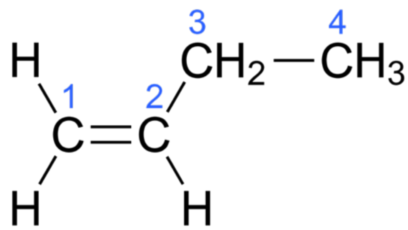
Pentane ($C_5H_{12}$)



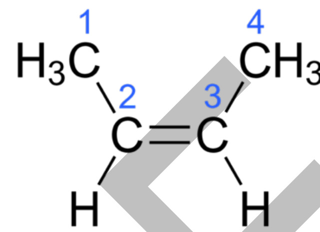
Methylbutane ($C_5H_{12}$)

**Position isomers**

- Position isomers are molecules with the same molecular formula and functional group, but the position of the functional group is different.
- For example, 1-butene and 2-butene both have the same molecular formula $C_4H_8$ but the position of the double bond is found in different positions.



1-butene ($C_4H_8$)

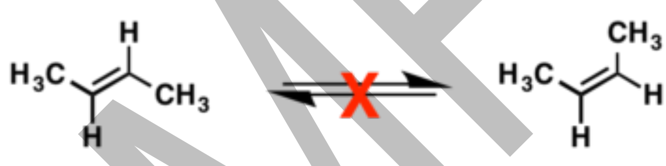


2-butene ($C_4H_8$)

**Geometric isomers**

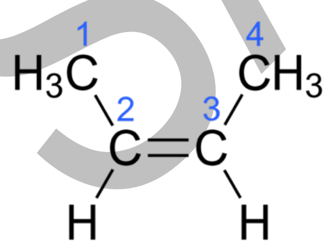
- Geometric isomers are molecules with the same molecular formula, functional group, number of carbons in the longest chain, but occupy different geometry in three-dimension space.

- In hydrocarbons, geometric isomers only exist for alkenes because pi-bonds cannot rotate about their own axis without disrupting the overlapping *p* orbitals of adjacent carbon atoms.

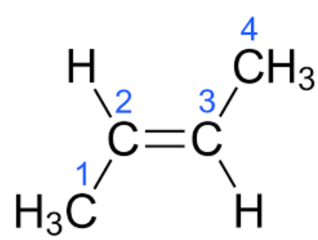



- Geometric isomers do not apply for alkynes because carbon atoms that form a triple bond exist in a linear conformation.

- ***Cis/trans* isomerism**
  - When non-hydrogen atoms are on the same side of the C=C bond, the '*cis*' prefix is added.
  - When non-hydrogen atoms are on the opposite side of the C=C bond, the '*trans*' prefix is added.



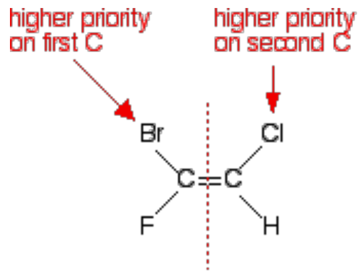
*cis*-2-butene ($C_4H_8$)



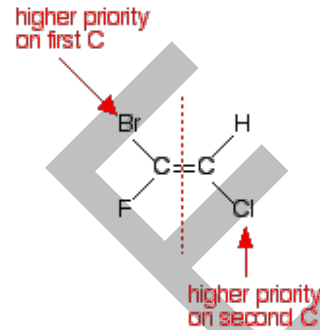
*trans*-2-butene ($C_4H_8$)

- **E/Z isomerism** is a better naming convention than the cis/trans convention because it always works. When there are more than two non-hydrogen substituents connected to a double C=C bond, cis/trans notation no longer works.

- Atoms which are adjacent to the carbons in the C=C bond are assigned priorities in the order of their atomic number.
- If on the two ends of the C=C bond, higher priority atoms are positioned on the same side, (*Z*) is assigned as a prefix.
- If on the two ends of the C=C bond, higher priority atoms are positioned on the opposite side, (*E*) is assigned as a prefix.




(*Z*)-1-bromo-2-chloro-1-fluoro-ethene



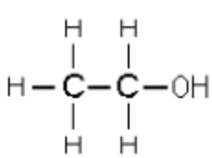

(*E*)-1-bromo-2-chloro-1-fluoro-ethene

**Functional group isomers**

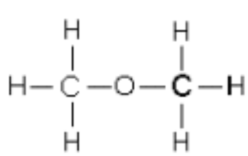
- Functional group isomers are molecules with the same molecular formula, but different functional groups.
- Hydrocarbons cannot have functional group isomers. There are three pairs of functional groups which typically have functional isomers:

- Ethers and alcohols

ethanol

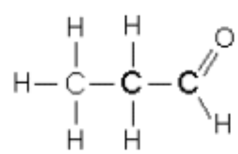


methoxymethane

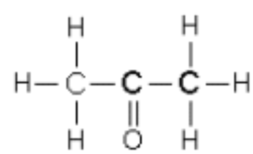


- Ketones and aldehydes

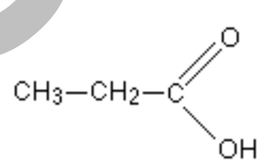
propanal



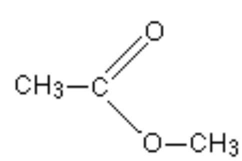
propanone (acetone)



- Carboxylic acids and esters.



propanoic acid



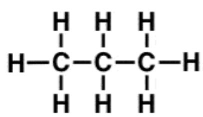
methyl ethanoate

## Molecular formula vs Structural formula

- Molecular formula informs about the composition of a molecule but does not disclose information about its structure and how the atoms are arranged.
  - Using molecular formula alone, isomers cannot be distinguished.

**Structural formula**

- There are three types of structural formulae all of which provide information on the exact structural identity of an organic molecule.



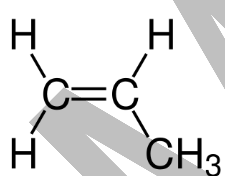
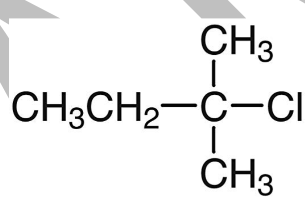
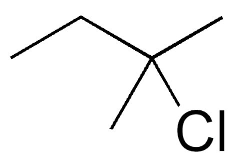
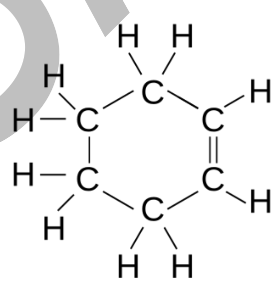
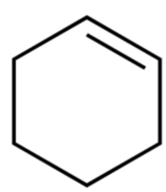
*Structural Formula*

*Line Diagram*
*(aka Skeletal formula)*

$CH_3CH_2CH_3$

*Condensed Formula*

- In the line diagram, the lines join carbon atoms and hydrogen atoms which are connected to carbon are not shown so it is important to know how many hydrogens are attached to each carbon.

| *Compound* | *Expanded form* | *Line diagram* | *Condensed formula* |
|---|---|---|---|
| propene |  |  | $CH_2CHCH_3$ |
| 2-chloro-2-methylbutane |  |  | $CCl(CH_3)_2CH_2CH_3$ |
| cyclohexene |  |  | $CHCHCH_2CH_2CH_2CH_2$ |

## Common uses of hydrocarbons in society

- Alkanes are commonly used as
  - fuels – methane (natural gas), propane and butane in LPG, octane in petrol, longer chain alkanes in aviation fuel and diesel.
  - Solvents: e.g. pentane and hexane to dissolve non-polar substances
  - long-chain alkanes are used in waxes and in bitumen.

- Alkenes are used in the chemical industry due to the reactivity of the C=C bond.
  - Ethylene (IUPAC name: ethene) can be converted into ethanol, haloalkanes, addition polymers, etc. Polymers such as polyethylene, polystyrene and PVC are derivatives of ethylene. These polymers have numerous uses for construction, insulation, toys, food wraps, etc.

- Alkynes are also reactive in nature due to their triple carbon-to-carbon bond.
  - ethyne (preferred name acetylene) is used as a fuel for welding.
  - Alkynes are commonly used as starting molecules for the synthesis of many pharmaceutical drugs.

## Disposal of hydrocarbons

- Organic substances cannot be poured down the drain and should be disposed separately in the 'Organic Liquid' waste container located in the fume hood. This is because:
  - Hydrocarbons are volatile and combustible (flammable), so they easily vaporise and burn to generate heat.
  - Hydrocarbon fumes may be toxic.
  - Incomplete combustion of hydrocarbons produces carbon monoxide, CO, which is odourless and toxic. Any combustion reactions involving hydrocarbons must be conducted in the fume hood.

- Halogenated hydrocarbons are required to be disposed in 'Halogenated Organic Waste' container because they are toxic upon inhalation and ingestion.
  - This includes any compounds that contain F, Cl, Br and I.

## Extraction of hydrocarbons from Earth

- Hydrocarbons – mainly alkanes – are extracted from crude oil/petroleum which forms in oil reservoirs within the Earth's crust.

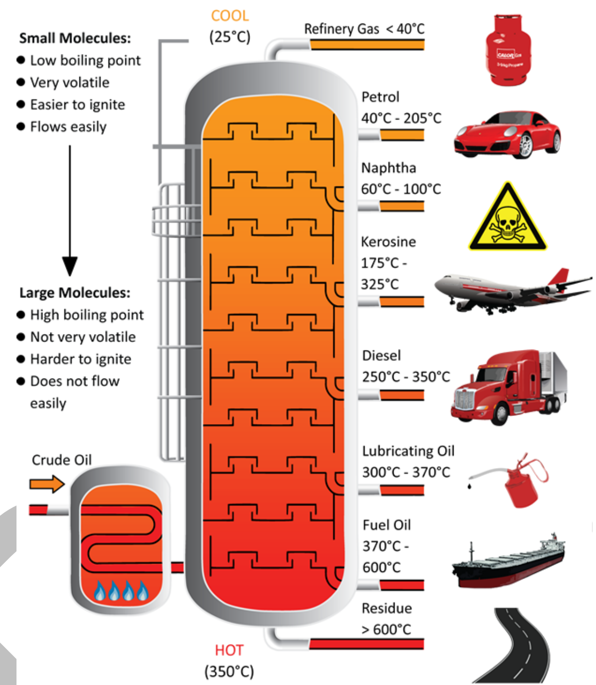
- **Detection**
  Geologists use seismic surveys to search for geological structures that may form oil reservoirs. The "classic" method includes making an underground explosion nearby and observing the seismic response that provides information about the geological structures under the ground.

- **Extraction**
  Extracting crude oil normally starts with drilling wells into an underground reservoir. The crude oil then undergoes **fractional distillation**, to separate the various components of the mixture into their useful fractions, based on boiling point and chain length.

- **Separation**
  Crude oil is passed through the bottom of a fractional distiller where the temperature is at its highest. Large hydrocarbons (higher boiling point) will condense into liquid form while smaller hydrocarbons remain as gases and ascend through the distiller.

  As gaseous hydrocarbons ascend, temperature starts decrease which means condensation occurs for the remaining molecules.

Fractional Distillation of Crude Oil



**Analyse the environmental, economic and sociocultural implications of obtaining and using hydrocarbons over the twentieth century.**

During the twentieth century, the world population increased significantly. With this increase in population came increased demands for materials such as fuels for transport, industry and heating, materials for construction to replace and supplement timber and iron, fibres for clothing and household goods and chemicals to improve medical care. For a large part of that century, the demands were satisfied by hydrocarbons in fossil fuels.

Coal provided a major source of energy for transport, for industry and for domestic heating. Coal gas also provided energy for cooking and heating. As the demands for liquid fuels for transport increased, crude oil refining increased, and petroleum provided not only petrol, diesel and aviation fuel but also chemicals such as ethylene.

Chemical industries based around fossil fuels developed. These included manufacture of polymers, such as polyethylene, PVC and polystyrene, as well as synthetically produced materials including esters, acids, alcohols, nylon, polyesters, synthetic rubber, adhesives, resins, medications, etc. These chemicals, based on the petroleum industry, changed the lifestyles of society but many of these chemicals had negative impacts on the environment, due to lack of biodegradability.

The exponential use of petroleum led to dwindling supplies and high costs of this non-renewable fossil fuel and by the 1970s it became evident that traditional materials needed to be supplemented or replaced by others derived from renewable resources. Electrical energy, once largely provided by the burning of fossil fuels such as coal in power stations, is now supplemented by the use of batteries and the development of the renewable energy industry. The development of materials used in medicine has been driven by improvements in understanding of health issues and research into new techniques.

As the world population continues to increase, as food supplies dwindle and as the demands for high quality health care, housing, transport and new technologies grow, there will be continued problems for the environment associated with these changes. Issues associated with climate change, related to the use of carbon-based fuels, need resolution in the short-term, as will the decreasing supplies of the non-renewable resources upon which chemical industry is still dependent. The use of renewable solar, wind, wave and geothermal power sources will become more significant, with the possibility of nuclear energy being harnessed safely for future generations. New sources of raw chemicals for the new technologies and industries of the future will need to be developed and these will continue to need further research and development of chemistry.