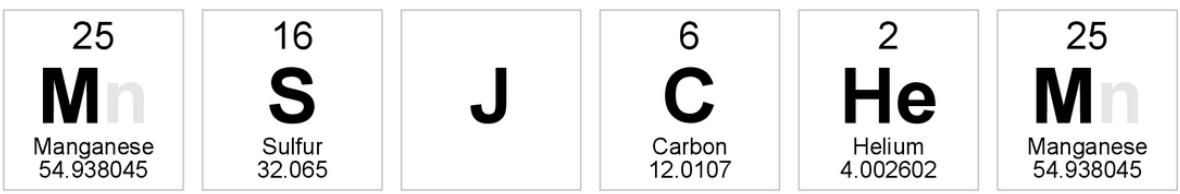
# Structure 3.2

IB CHEMISTRY SL



**Structure 3.2.1**

**Understandings:**

- Organic compounds can be represented by different types of formulas. These include empirical, molecular, structural (full and condensed), stereochemical and skeletal.

**Learning outcomes:**

- Identify different formulas and interconvert molecular, skeletal and structural formulas.
- Construct 3D models (real or virtual) of organic molecules.

**Additional notes:**

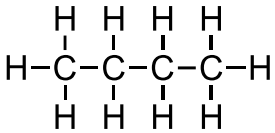
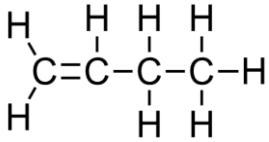
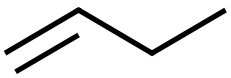
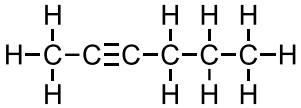
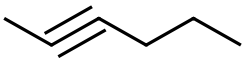
- Stereochemical formulas are not expected to be drawn, except where specifically indicated.

**Linking questions:**

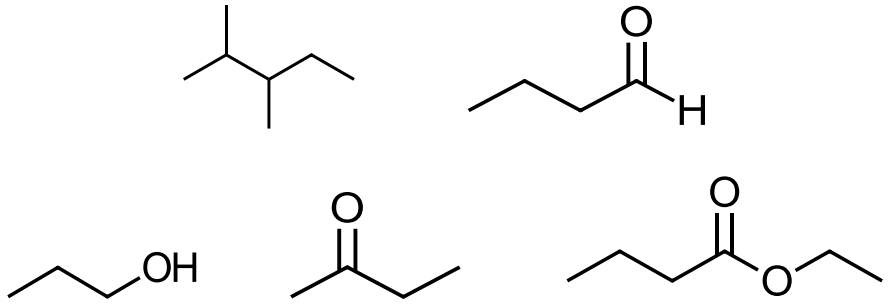
- Structure 2.2 What is unique about carbon that enables it to form more compounds than the sum of all the other elements' compounds?

## Structural formulae

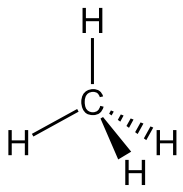
- The different types of formulas used in organic chemistry are shown below.

| Compound | Molecular formula | Empirical formula | Full structural formula | Condensed structural formula | Skeletal formula |
|---|---|---|---|---|---|
| Butane | $C_4H_{10}$ | $C_2H_5$ |  | $CH_3(CH_2)_2CH_3$ |  |
| But-1-ene | $C_4H_8$ | $CH_4$ |  | $CH_2CHCH_2CH_3$ |  |
| Hex-2-yne | $C_6H_{10}$ | $C_3H_5$ |  | $CH_3CCCH_2CH_2CH_3$ |  |

**Skeletal formulae**




**Stereochemical formulae**




- The two solid lines are in the plane of the paper.
- The wedge is coming out from the plane of the paper.
- The dashed line is going into the plane of the paper.

**Structure 3.2.2**

**Understandings:**

- Functional groups give characteristic physical and chemical properties to a compound. Organic compounds are divided into classes according to the functional groups present in their molecules.

**Learning outcomes:**

- Identify the following functional groups by name and structure: halogeno, hydroxyl, carbonyl, carboxyl, alkoxy, amino, amido, ester, phenyl.

**Additional notes:**

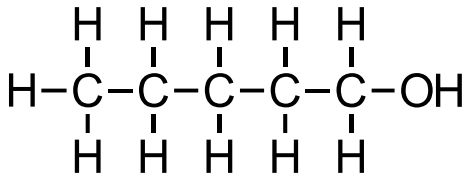
- The terms “saturated” and “unsaturated” should be included.

**Linking questions:**

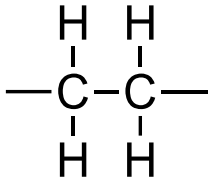
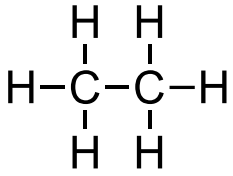
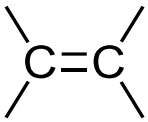
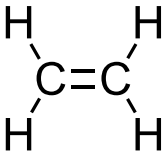
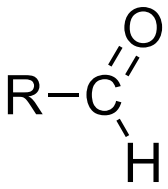
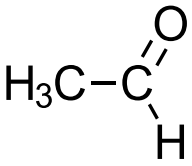
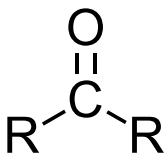
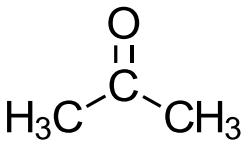
- Structure 2.4 (HL) What is the nature of the reaction that occurs when two amino acids form a dipeptide?

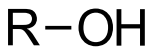
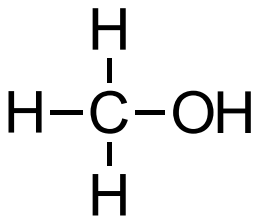
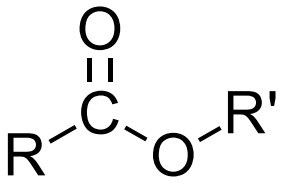
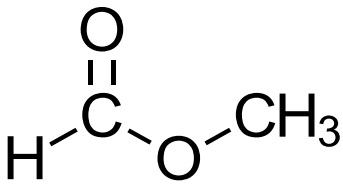
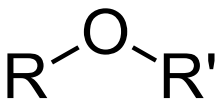
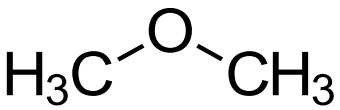
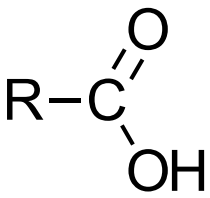
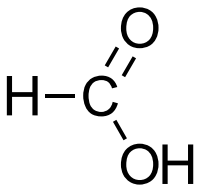
**Functional groups**

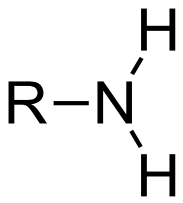
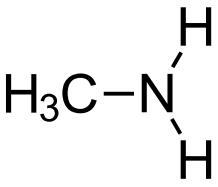
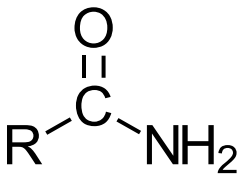
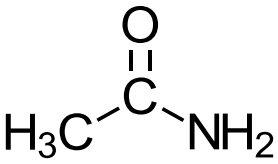
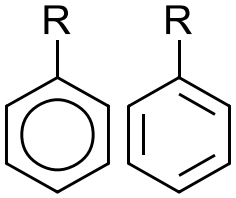
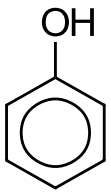
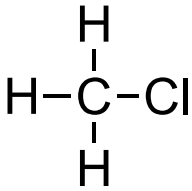
- A functional group is a group of atoms within a molecule that are responsible for the characteristic chemical reactions of the molecule.



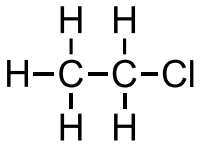
Class: alcohol
Functional group: hydroxyl group

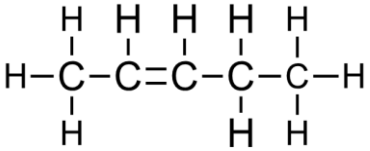
| Class | Functional group name | Structural formula | Example |
|---|---|---|---|
| **Alkane** | |  |  **Ethane $CH_3CH_3$** |
| **Alkene** | |  |  **Ethene $C_2H_4$** |
| **Alkyne** | |  |  **Ethyne CHCH** |
| **Aldehyde** | **Carbonyl** |  R-CHO |  **Ethanal $CH_3CHO$** |
| **Ketone** | **Carbonyl** |  R-CO-R' |  **Propanaone $CH_3COCH_3$** |

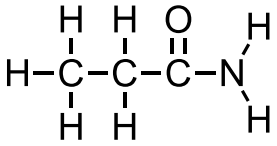
| Class | Functional group name | Structural formula | Example |
|---|---|---|---|
| **Alcohol** | **Hydroxyl** |  |  **Methanol $CH_3OH$** |
| **Ester** | **Ester** |  R-COO-R' R-$CO_2$-R' |  **Methyl methanoate $HCOOCH_3$ or $HCO_2CH_3$** |
| **Ether** | **Alkoxy** |  R-O-R' |  **Methoxymethane $CH_3OCH_3$** |
| **Carboxylic acid** | **Carboxyl** |  R-COOH $R-CO_2H$ |  **Methanoic acid $HCOOH$ or $HCO_2H$** |

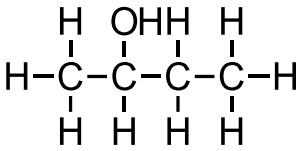
| Class | Functional group name | Structural formula | Example |
|---|---|---|---|
| **Amine** | **Amino** |  **R-NH$_2$** |  **Methanamine** **CH$_3$NH$_2$** |
| **Amide** | **Amido** |  **R-CONH$_2$** |  **Methanamide** **CH$_3$CONH$_2$** |
| **Arene** | **Phenyl** |  **C$_6$H$_5$-** |  **Phenol** **C$_6$H$_5$OH** |
| **Halogenoalkane** | **Fluoro-**<br>**Chloro-**<br>**Bromo-**<br>**Iodo-**<br><br>**where X is a F, Cl, Br or I atom** | R-X |  **Chloromethane** **CH$_3$Cl** |

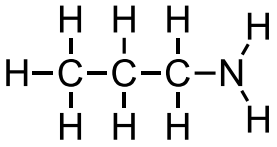
**Exercise**: For each of the following organic compounds, state the class and functional group.

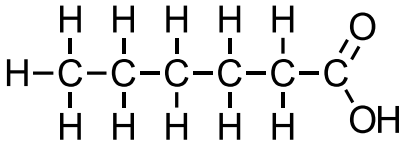


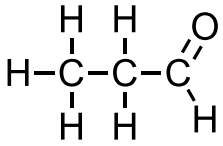


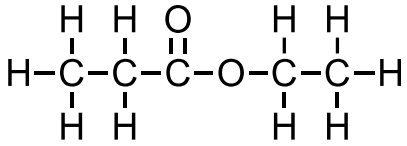


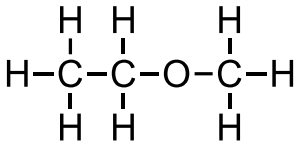


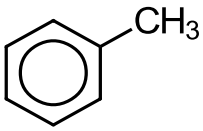


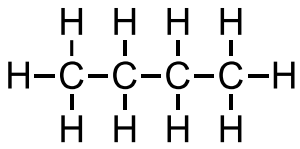




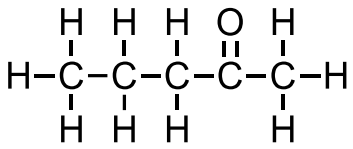












**Structure 3.2.3 and 3.2.4**

**Understandings:**

- A homologous series is a family of compounds in which successive members differ by a common structural unit, typically $CH_2$. Each homologous series can be described by a general formula (3.2.3).
- Successive members of a homologous series show a trend in physical properties (3.2.4).

**Learning outcomes:**

- Identify the following homologous series: alkanes, alkenes, alkynes, halogenoalkanes, alcohols, aldehydes, ketones, carboxylic acids, ethers, amines, amides and esters (3.2.3).
- Describe and explain the trend in melting and boiling points of members of a homologous series (3.2.4).

**Additional notes:**

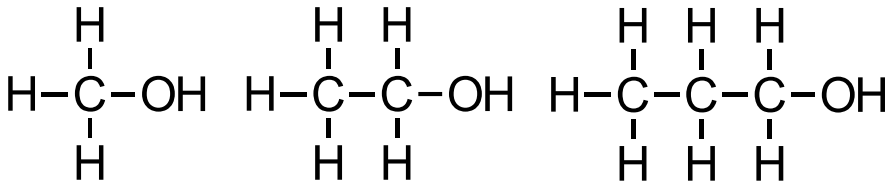
- The terms “saturated” and “unsaturated” should be included.

**Linking questions:**

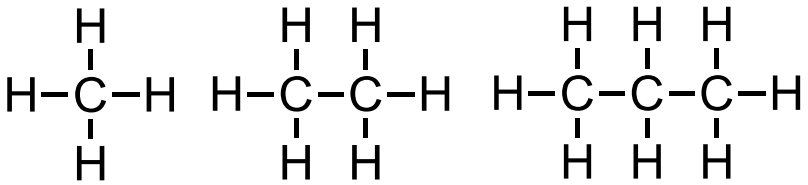
- Structure 2.4 (HL) What is the nature of the reaction that occurs when two amino acids form a dipeptide?
- Structure 2.2 What is the influence of the carbon chain length, branching and the nature of the functional groups on intermolecular forces?

**Homologous series**

- A homologous series is a series of organic compounds of the same family which differ by a common structural unit ($CH_2$).



- Functional group: hydroxyl (OH) – each member differs by a $CH_2$ group.
- Members of a homologous series have similar chemical properties.



- Members of a homologous series show a gradation in physical properties (such as the increasing boiling point of the alkanes).
- They also have the same general formula.

**Summary:** Members of a homologous series:

- differ by a $CH_2$
- have the same general formula
- have similar chemical properties
- show a gradation (gradual increase) in physical properties such as boiling point
- have the same functional group

## Factors that affect the boiling points of organic compounds

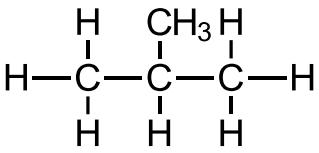
### Molar mass and boiling point

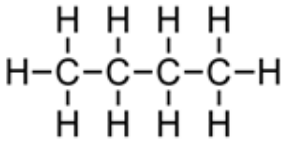
| alkane | molar mass ($gmol^{-1}$) | boiling point (°C) |
|---|---|---|
| methane | 16 | -164 |
| ethane | 30 | -89 |
| propane | 44 | -42 |
| butane | 58 | -0.5 |
| pentane | 72 | 36 |
| hexane | 86 | 69 |
| heptane | 100 | 98 |
| octane | 114 | 125 |
| nonane | 128 | 151 |
| decane | 142 | 174 |

- As the molar mass of the compound increases, the boiling point increases.
- As the molar mass increases, the strength of the London dispersion forces between the molecules increases (the molecules have more electrons and are more easily polarisable).
- More energy is required to overcome the London dispersion forces between the molecules, therefore, the boiling point increases.

### Branched chain isomers vs straight chain isomers

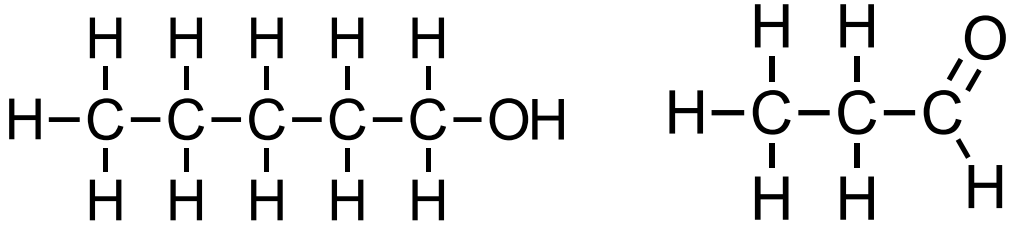
- Branched-chain isomers have lower boiling points than straight-chain isomers.
- The branches reduce the contact surface area between the molecules which reduces the strength of the London dispersion forces between the molecules and lowers the boiling point.
- The structures of 2-methylpropane (boiling point -11.7 °C) and butane (boiling point -1 °C) are shown below.



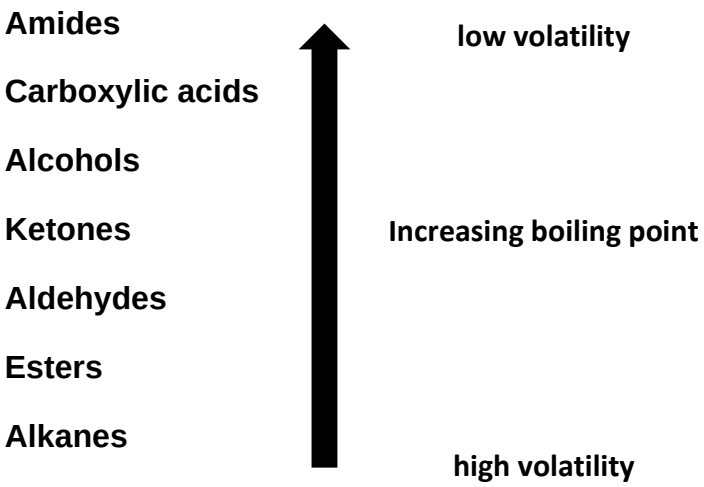


- 2-methylpropane, a branched alkane, has a lower boiling than butane.
- The branches result in a lower contact surface area between the molecules.

**Effect of functional group**



- Compounds with functional group containing H bonded to O or N have hydrogen bonding between their molecules.
- Compounds with functional group containing carbonyl group (C=O) have dipole-dipole forces between their molecules.
- Alcohols, amides and carboxylic acids have higher boiling points as they are able to form hydrogen bonds between their molecules.
- Aldehydes, ketones, and esters have dipole-dipole forces between their molecules.
- Alkanes, alkenes and alkynes have London dispersion forces between their molecules.



**Exercises:**

1. Methane and heptane belong to the same class (the alkanes). Predict and explain which compound has a higher boiling point.

2. Explain the difference in boiling point between the structural isomers pentane and 2-methylbutane.

3. Ethanol and propane have similar molar masses but different boiling points. Predict and explain which compound has the highest boiling point.

**Structure 3.2.5**
**Understandings:**

- IUPAC nomenclature refers to a set of rules used by the International Union of Pure and Applied Chemistry to apply systematic names to organic and inorganic compounds.

**Learning outcomes:**

- Apply IUPAC nomenclature to saturated or mono-unsaturated compounds that have up to six carbon atoms in the parent chain and contain one type of the following functional groups: halogeno, hydroxyl, carbonyl, carboxyl.

**Additional notes:**

- Include straight-chain and branched-chain isomers.

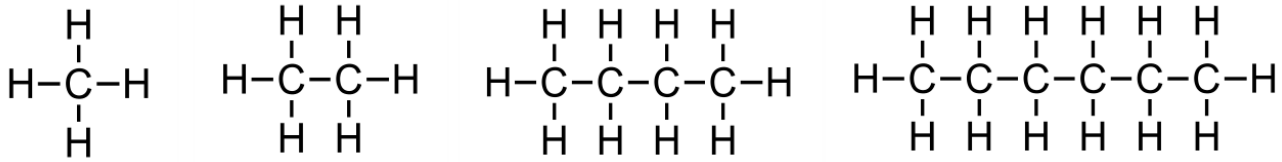
**Naming organic compounds**

- Students are required to name organic compounds with up to 6 carbon atoms in the longest chain.

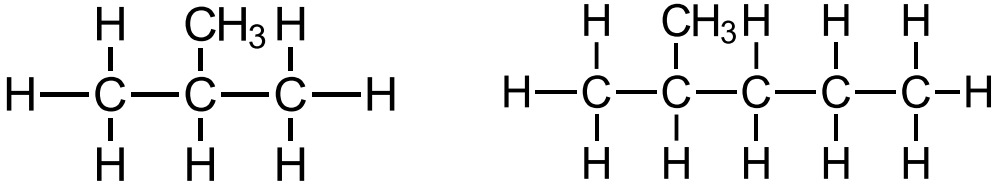
| number of carbon atoms | root / stem |
|---|---|
| 1 | meth- |
| 2 | eth- |
| 3 | prop- |
| 4 | but- |
| 5 | pent- |
| 6 | hex- |

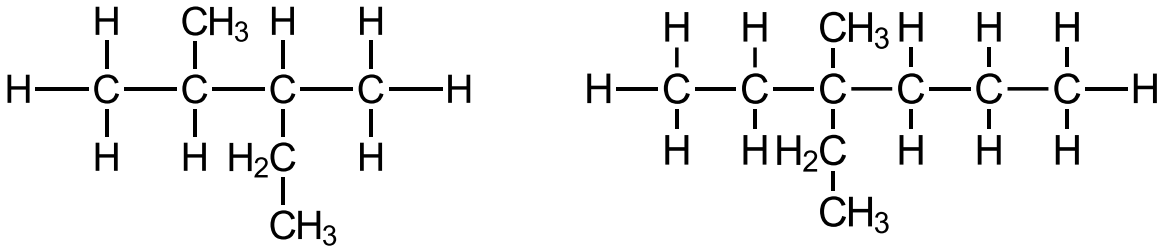
**Alkanes**

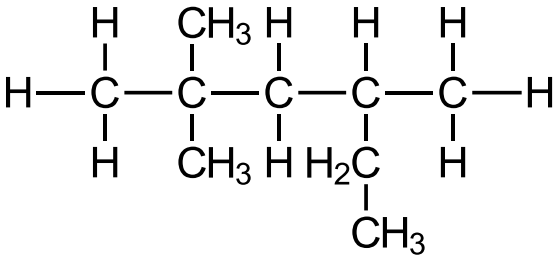
- General formula $C_nH_{2n+2}$
- Alkanes are saturated hydrocarbons (C-C single bonds).



**Branched-chain alkanes**

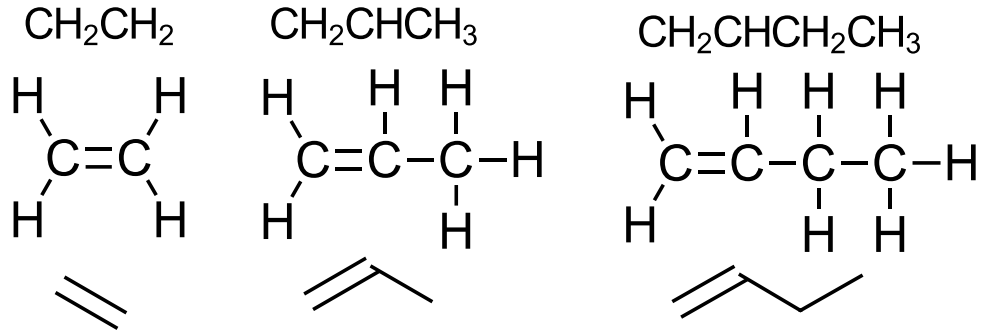


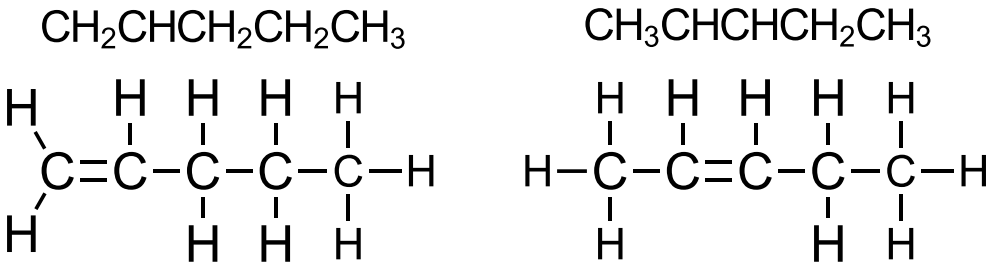




**Alkenes**

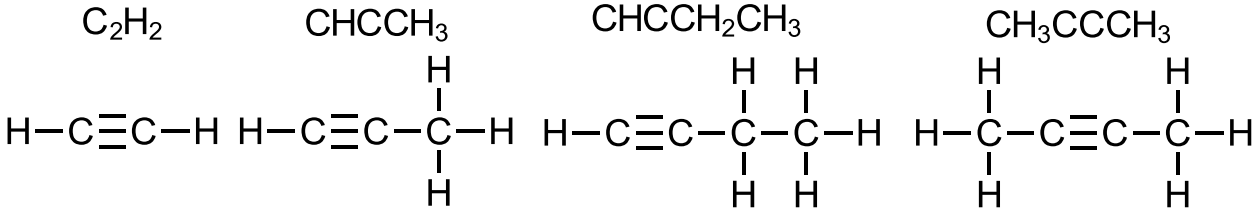
- General formula $C_nH_{2n}$
- Alkenes are unsaturated hydrocarbons (C=C double bond).

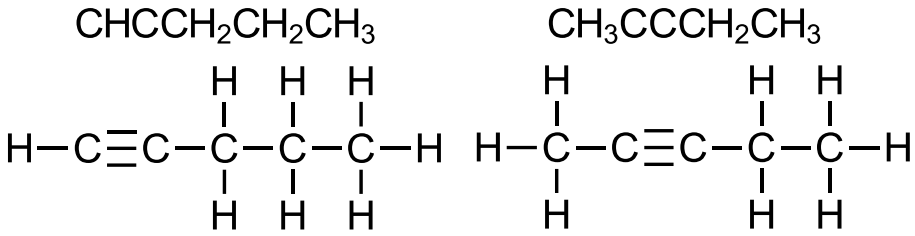




**Alkynes**

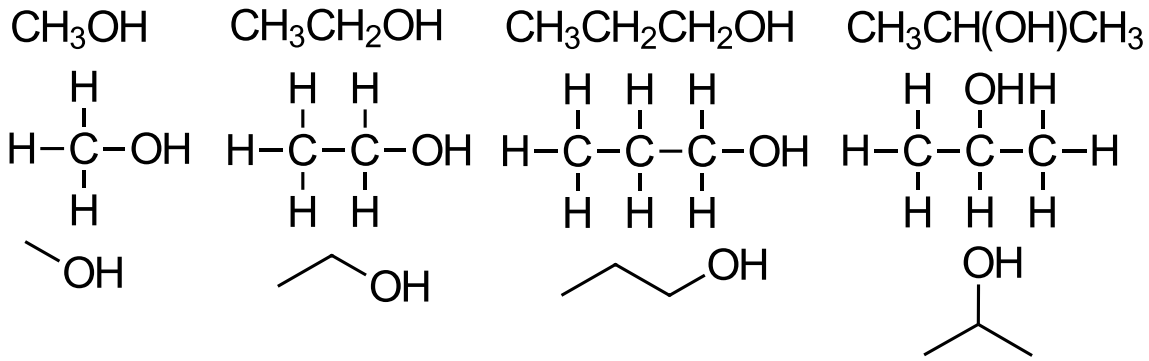
- General formula $C_nH_{2n-2}$
- Alkynes are unsaturated hydrocarbons (C to C triple bond).

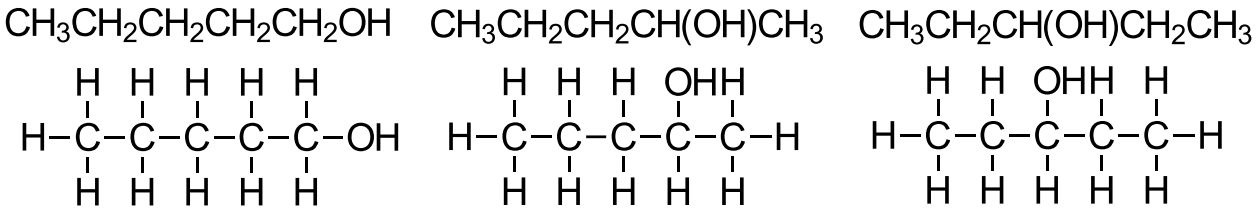




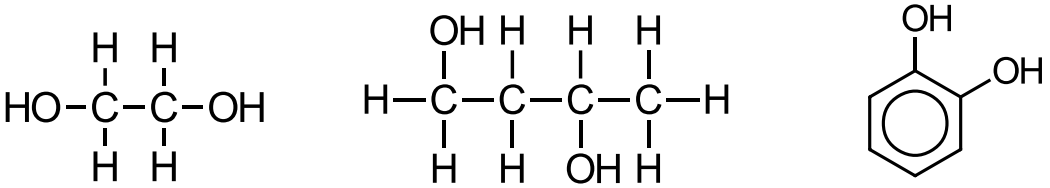

**Alcohols**

- General formula $C_nH_{2n+1}OH$



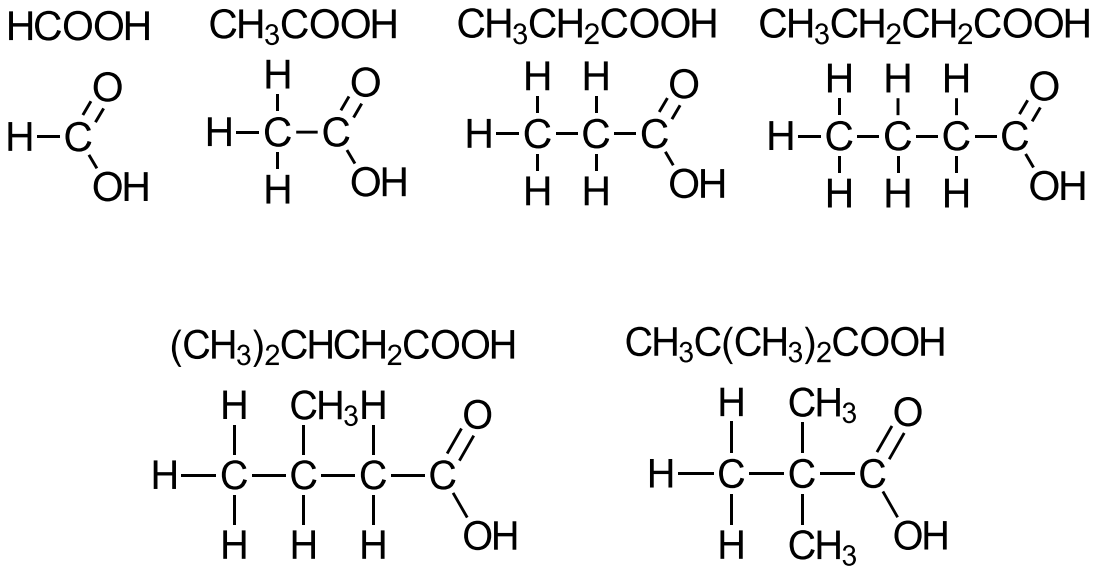




**Diols (compounds with two OH groups)**

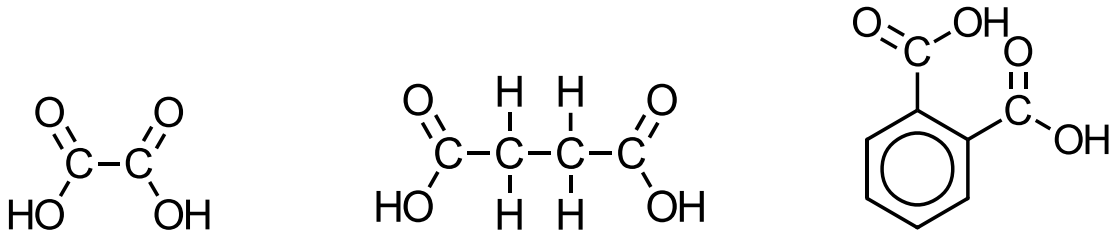


**Carboxylic acids (COOH or $CO_2H$)**

- General formula $C_nH_{2n+1}COOH$

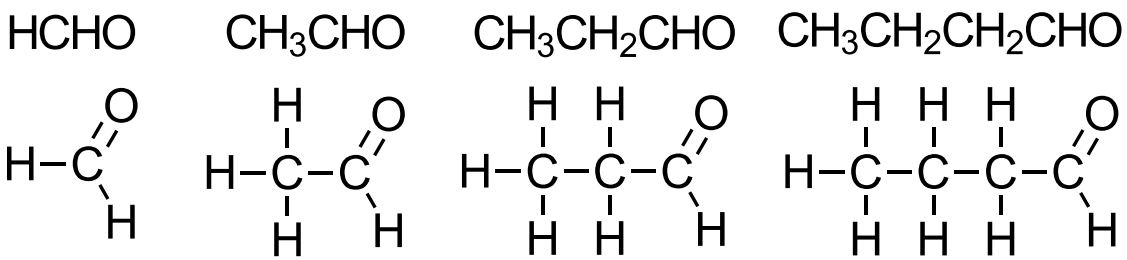



**Dicarboxylic acids (compounds with two carboxyl groups)**



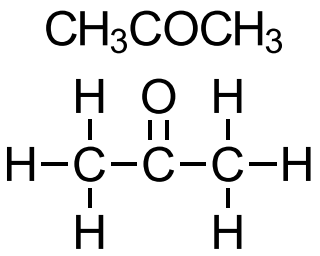
**Aldehydes**

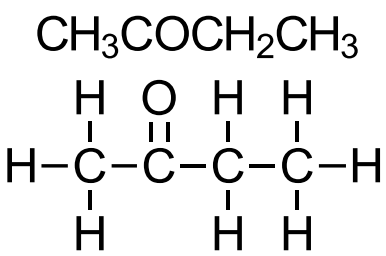
- General formula $C_nH_{2n}O$

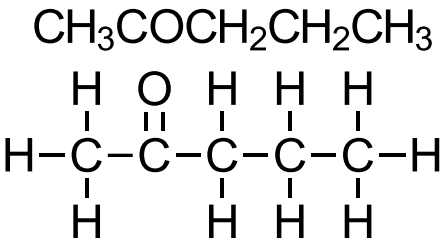


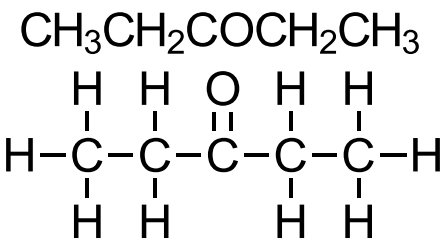
**Ketones**

- General formula $C_nH_{2n}O$



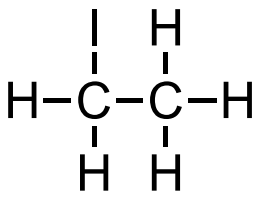


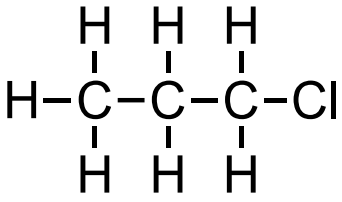


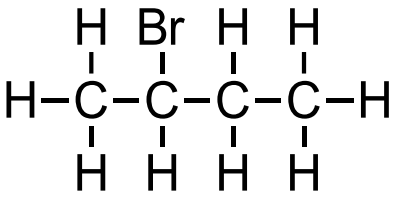


**Halogenoalkanes**

- Halogenoalkanes contain an atom of fluorine, chlorine, bromine or iodine.
- General formula $C_nH_{2n+1}X$

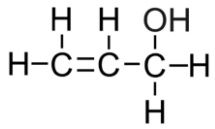




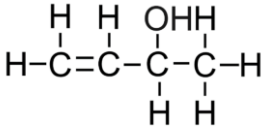


## Naming unsaturated compounds

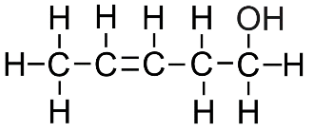
### Alcohols



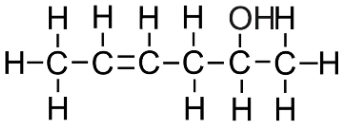
CHCHCH$_2$OH



CHCHCH(OH)CH$_3$

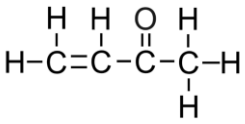


CH$_3$CHCHCH$_2$CH$_2$OH

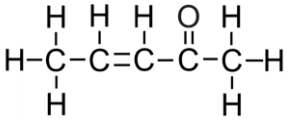


CH$_3$CHCHCH$_2$CH(OH)CH$_3$

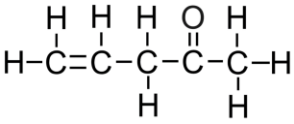
### Ketones



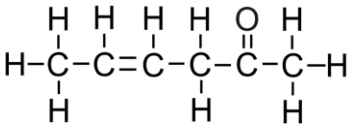
CHCHCOCH$_3$



CH$_3$CHCHCOCH$_3$

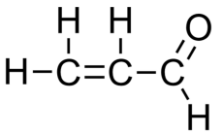


CH$_2$CHCH$_2$COCH$_3$

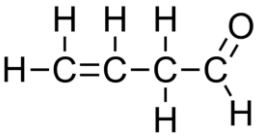


CH$_3$CHCHCH$_2$COCH$_3$

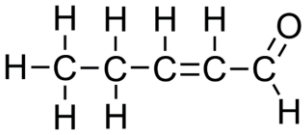
### Aldehydes



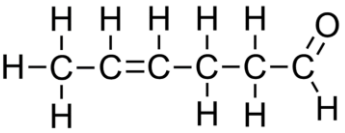
CHCHCHO



CH$_2$CHCH$_2$CHO

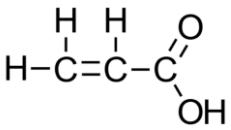


CH$_3$CH$_2$CHCHCHO

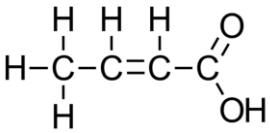


CH$_3$CHCHCH$_2$CH$_2$CHO

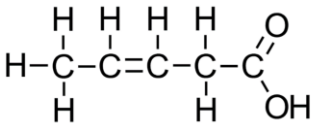
### Carboxylic acids



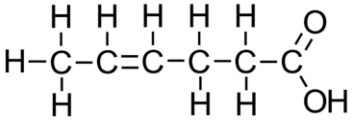
CH$_2$CHCO$_2$H



CH$_3$CHCHCO$_2$H

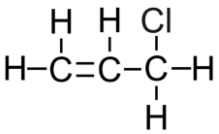


CH$_3$CHCHCH$_2$CO$_2$H

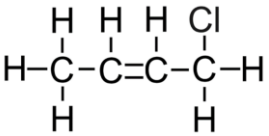


CH$_3$CHCHCH$_2$CH$_2$CO$_2$H

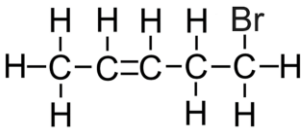
### Halogenoalkanes



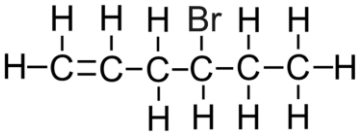
CH$_2$CHCH$_2$Cl



CH$_3$CHCHCH$_2$Cl



CH$_3$CHCHCH$_2$CH$_2$Br



CH$_2$CHCH$_2$CHBrCH$_2$CH$_3$

**Structure 3.2.6**

**Understandings:**

- Structural isomers are molecules that have the same molecular formula but different connectivities.

**Learning outcomes:**

- Recognise isomers, including branched, straight-chain, position and functional group isomers.

**Additional notes:**

- Primary, secondary and tertiary alcohols, halogenoalkanes and amines should be included.

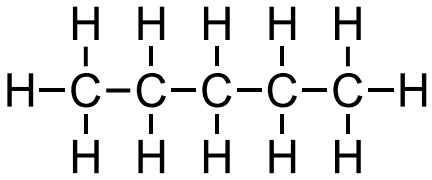
**Linking questions:**

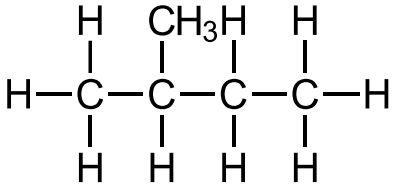
- Structure 2.2 (HL) How does the fact that there are only 3 isomers of dibromobenzene support the current model of benzene's structure?

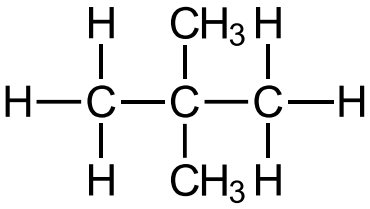
**Structural isomers**

- Structural isomers are compounds with the same molecular formula but different arrangements of atoms.
- They can be divided into branched, straight-chain, position and functional group isomers.

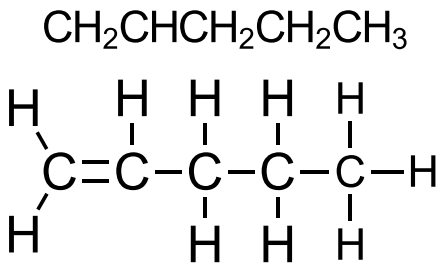
**Structural isomers of $C_5H_{12}$ (straight-chain and branched isomers)**

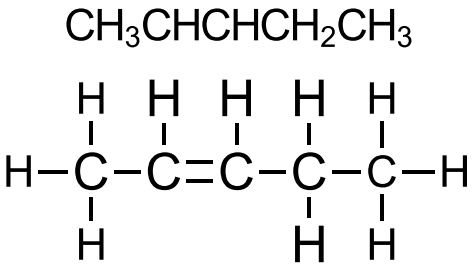




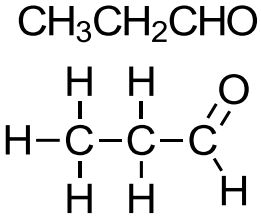


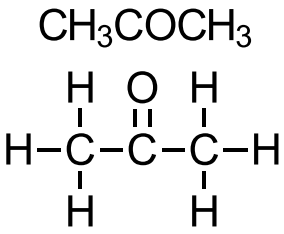
**Structural isomers of $C_5H_{10}$ (position isomers)**





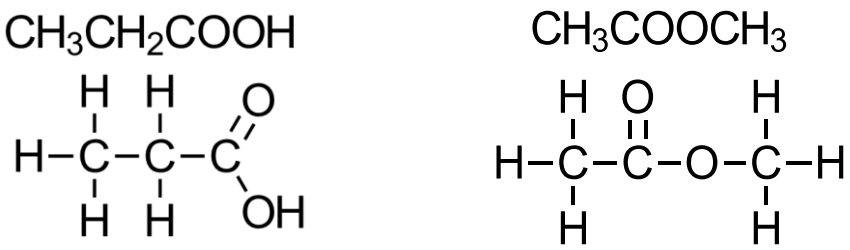
**Structural isomers of $C_3H_6O$ (functional group isomers)**



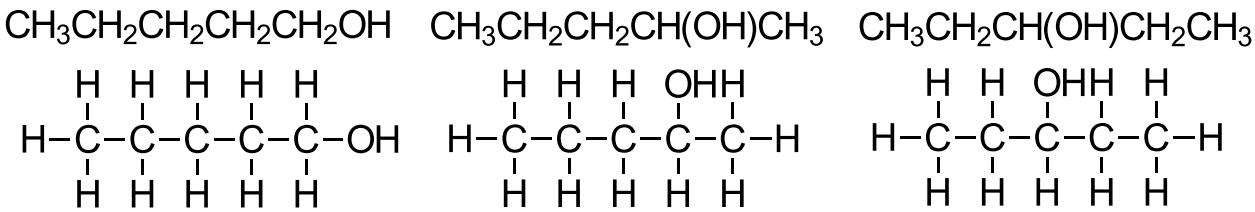


**Exercise:** Identify the type of isomerism shown by the following compounds.

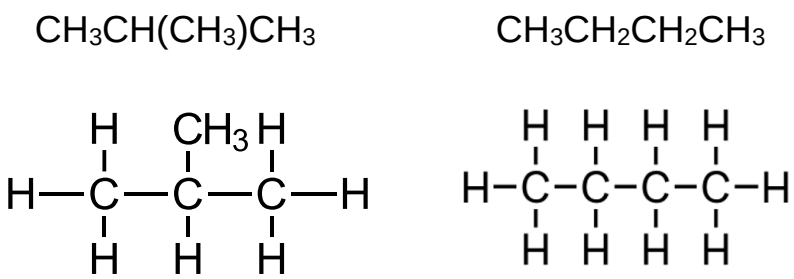
**1.** Structural isomers of $C_3H_6O_2$




**2.** Structural isomers of $C_5H_{12}O$

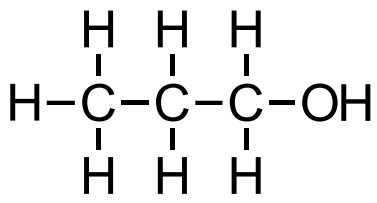
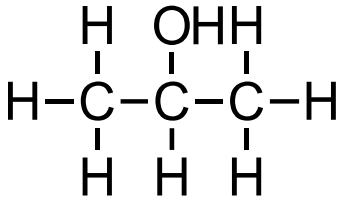
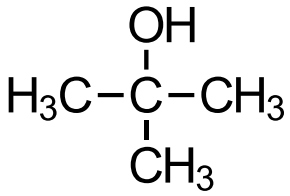



**3.** Structural isomers of $C_4H_{10}$



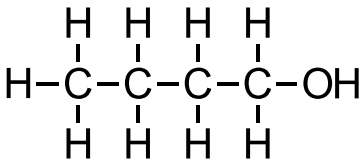
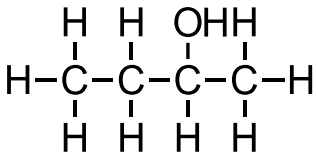
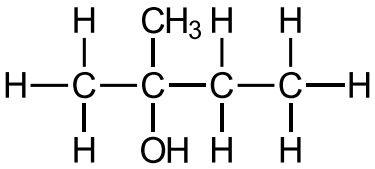
**Classification of organic compounds**

- Alcohols, amines and halogenoalkanes can be classified as primary, secondary or tertiary depending on how many carbons atoms are bonded to the carbon atom that is bonded directly to the functional group.

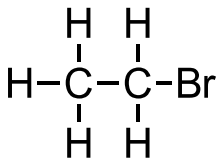
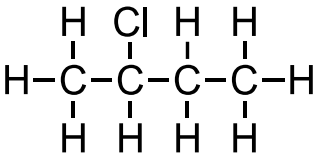
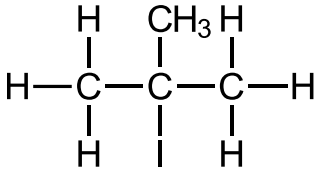




**Exercise:**

**1.** Name and classify the following alcohols as primary, secondary or tertiary.

**2.** Name and classify the following halogenoalkanes as primary, secondary or tertiary.

**3.** Classify the following amines as primary, secondary or tertiary.