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Chemistry

For the IB Diploma

> Chapter 11

Functional groups: Classification of organic compounds

> Homologous series

- A homologous series is a series of compounds with the same functional group, where each member differs from the next by $-\text{CH}_2-$.
- The homologous series can usually be described by a general formula, e.g., $\text{C}_n\text{H}_{2n+2}$ for alkanes.
- The members of the homologous series show similar chemical properties.
- The members of the homologous series show a gradation in physical properties, such as boiling point.

> Complete the table with different types of formulas for the members of the alkane homologous series

Name	Molecular formula	Empirical Formula	Structural formula	
			Condensed	Displayed formula
Methane				$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{H} \end{array}$
Ethane				$\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$
Propane				$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \text{H} \quad \text{H} \end{array}$
Butane				$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \quad \\ \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \end{array}$
Pentane				$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \quad \quad \\ \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \end{array}$
Hexane				$\begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \\ \quad \quad \quad \quad \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \quad \quad \quad \\ \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \quad \text{H} \end{array}$

The general formula of the alkane homologous series is $\text{C}_n\text{H}_{2n+2}$. What is the formula of the alkane with 25 C atoms?

> Representing molecules

stereochemical formula

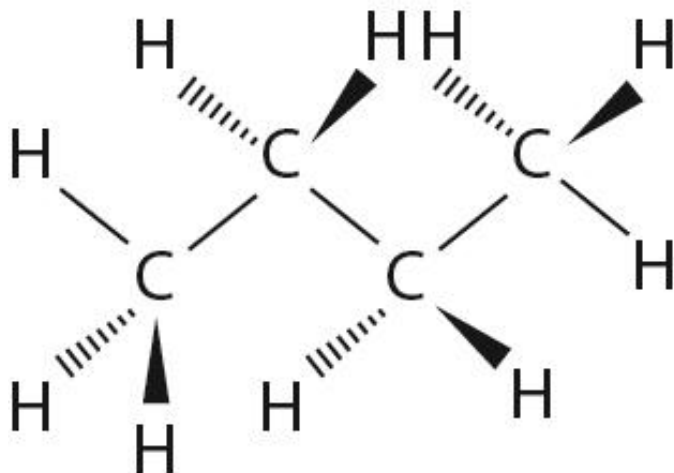


Figure 11.1: The stereochemical formula of butane showing the tetrahedral arrangement around the carbon atoms.

or **skeletal formula**

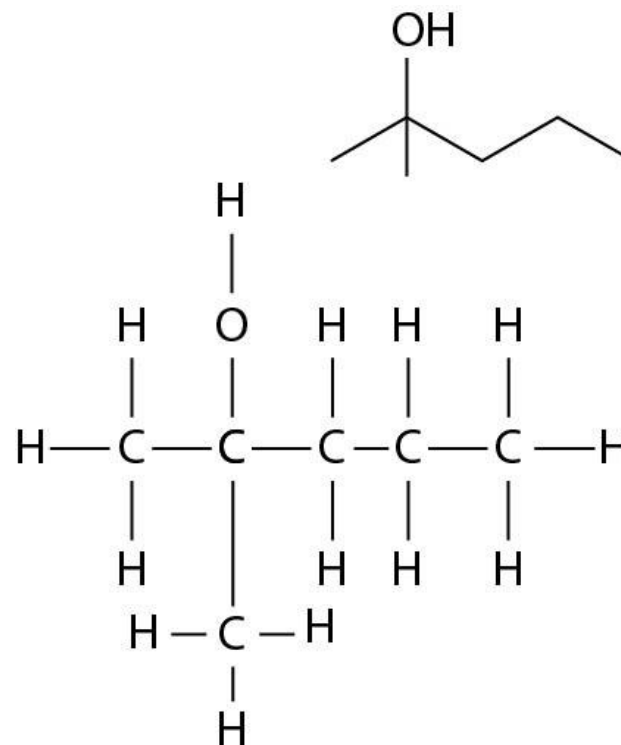


Figure 11.2: A skeletal formula and a displayed formula for 2-methylpentan-2-ol.

> Chain isomers

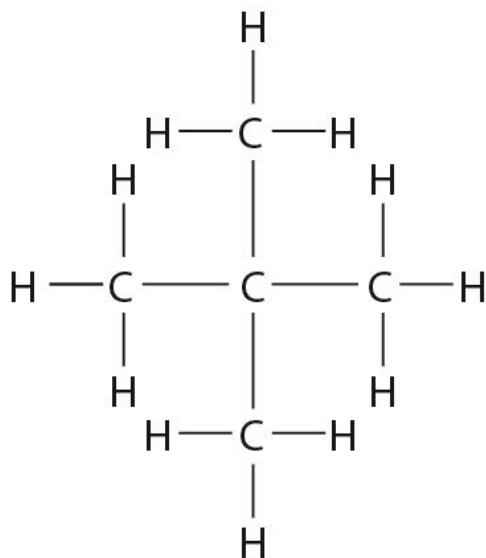
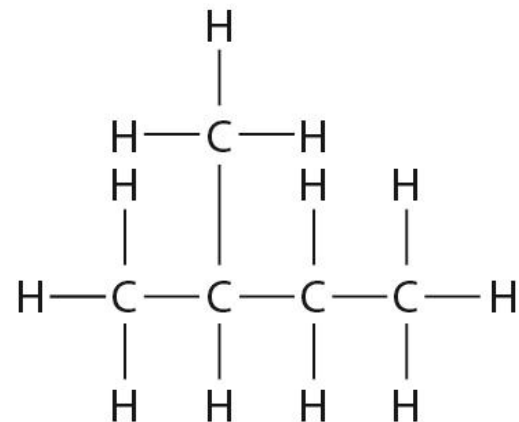
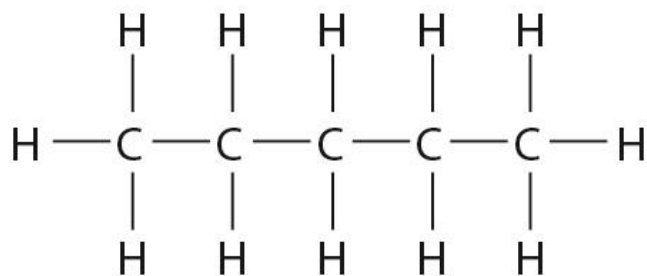


Figure 11.3: Structures of the isomers of C₅H₁₂.

> Some isomers of $C_5H_{12}O$

Structural isomers: two or more compounds that have the same molecular formula but different structural formulas; i.e., the atoms are joined together in a different way.

-OH attached to carbon 1	-OH attached to carbon 2	-OH attached to carbon 3
$ \begin{array}{ccccccc} & \text{OH} & \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \\ & & & & & & \\ \text{H} & -\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{C}-\text{H} \\ & & & & & & \\ & \text{H} & \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \end{array} $	$ \begin{array}{ccccccc} & \text{H} & \text{OH} & \text{H} & \text{H} & \text{H} & \text{H} \\ & & & & & & \\ \text{H} & -\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{C}-\text{H} \\ & & & & & & \\ & \text{H} & \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \end{array} $	$ \begin{array}{ccccccc} & \text{H} & \text{H} & \text{OH} & \text{H} & \text{H} & \text{H} \\ & & & & & & \\ \text{H} & -\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{C}-\text{H} \\ & & & & & & \\ & \text{H} & \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \end{array} $

Figure 11.4: Positional isomers

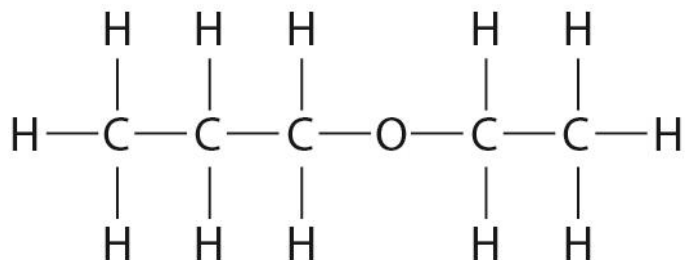


Figure 11.5: Functional group isomers

> Naming alkanes

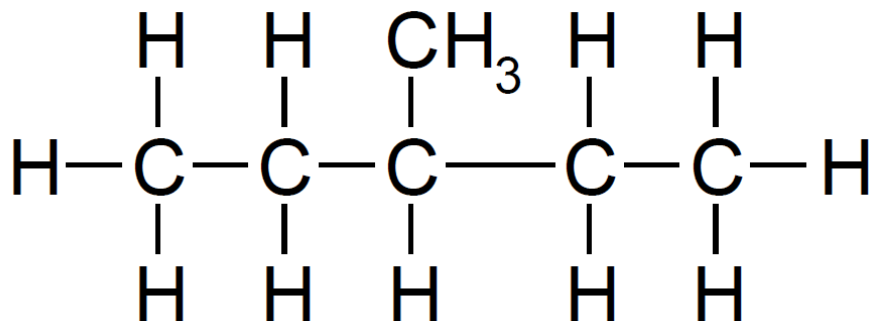


Figure 11.6: 3-methylpentane.

No. C atoms	Prefix
1	meth–
2	eth–
3	prop–
4	but–
5	pent–
6	hex–

–CH ₃	methyl
–C ₂ H ₅	ethyl
–C ₃ H ₇	propyl

> Naming alkenes

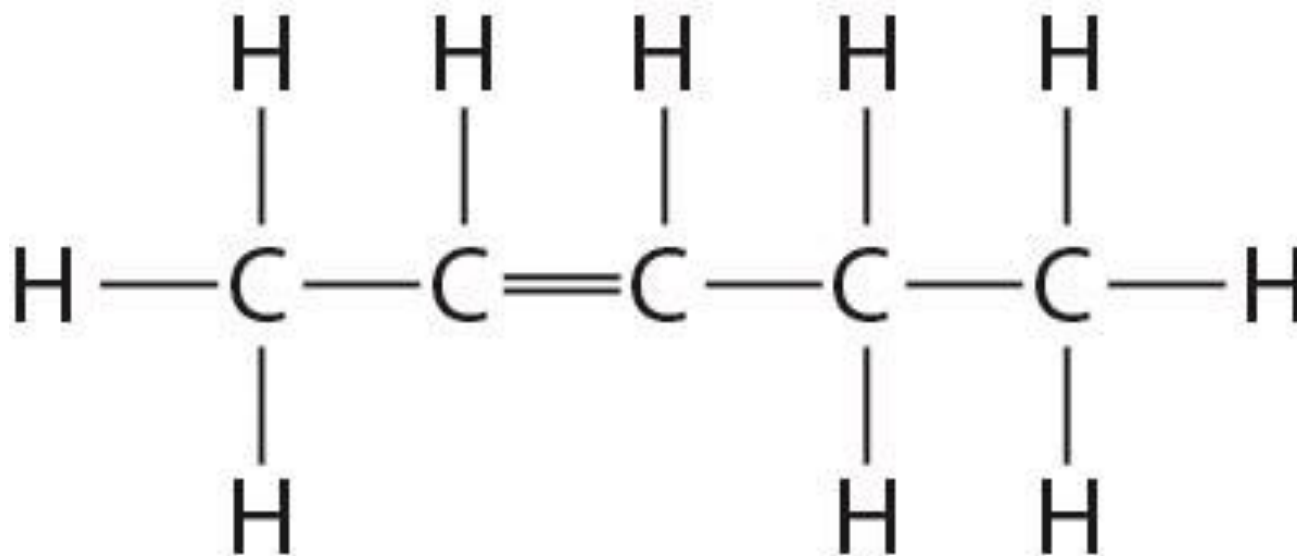


Figure 11.7: Pent-2-ene.

> Naming alcohols

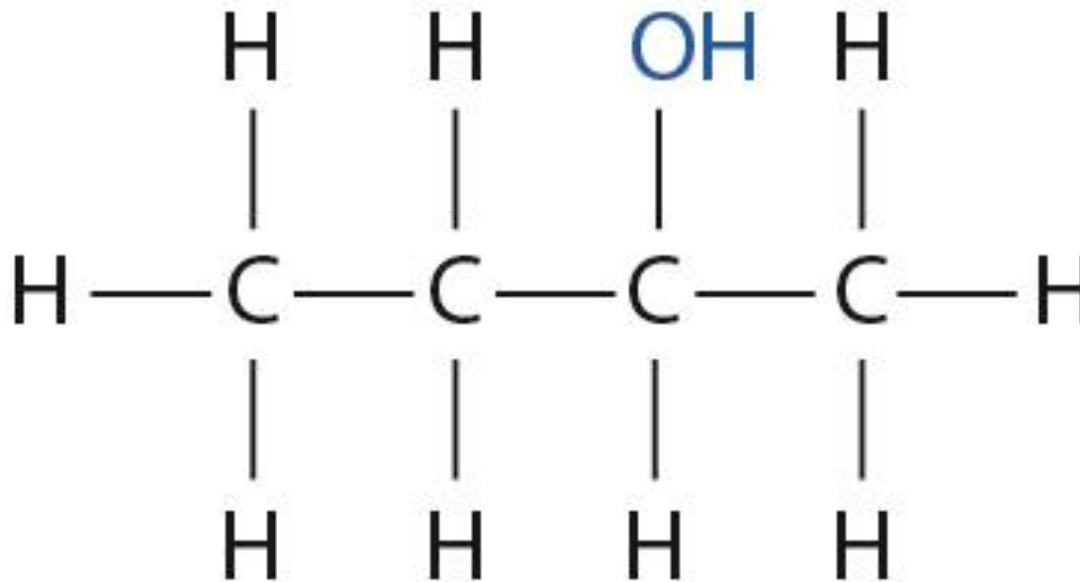


Figure 11.8: Butan-2-ol.

> Primary, secondary and tertiary alcohols

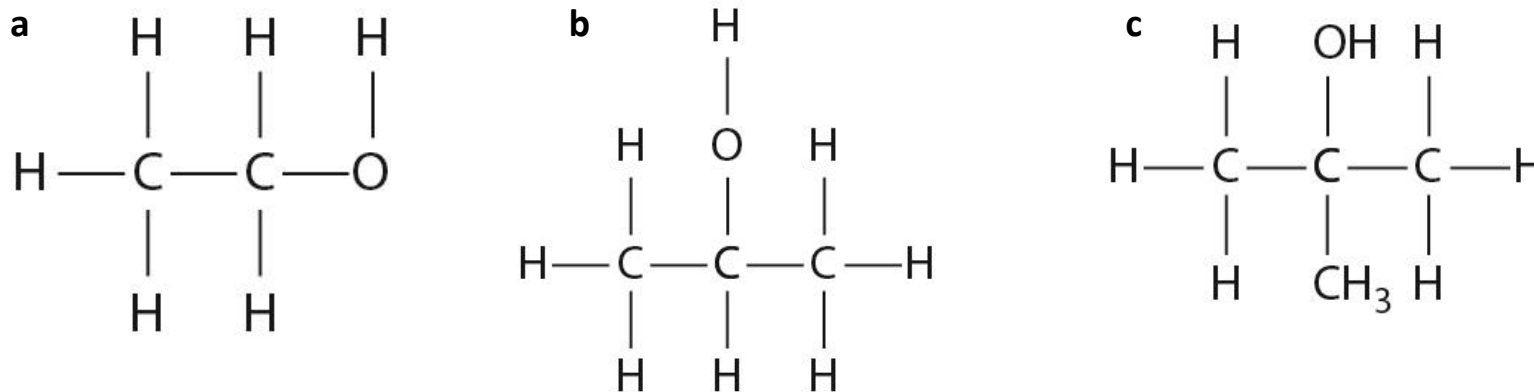


Figure 11.9: Examples of **a** primary, **b** secondary and **c** tertiary alcohols.

> Naming carbonyls

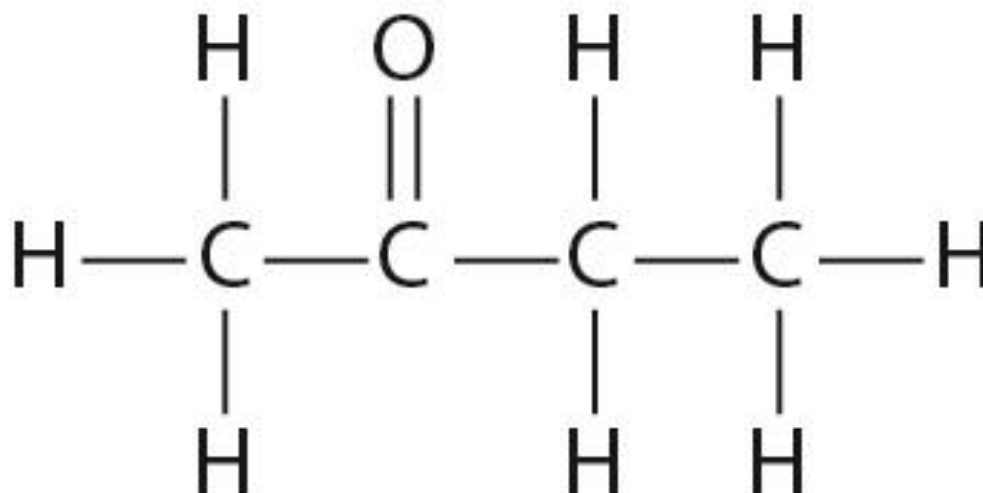


Figure 11.10: Butanone.

> Naming carboxylic acids

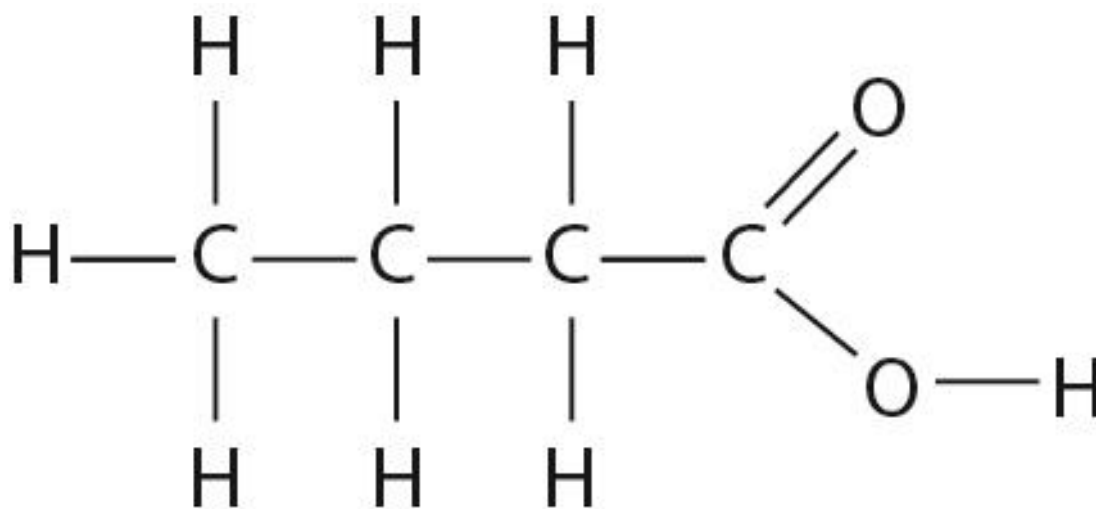


Figure 11.11: Butanoic acid.

> Carboxylic acids

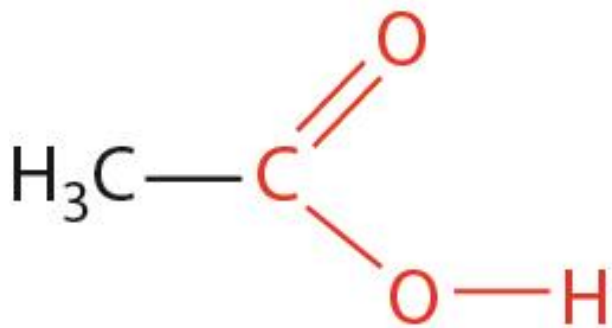


Figure 11.12: Different representations of the carboxyl functional group.

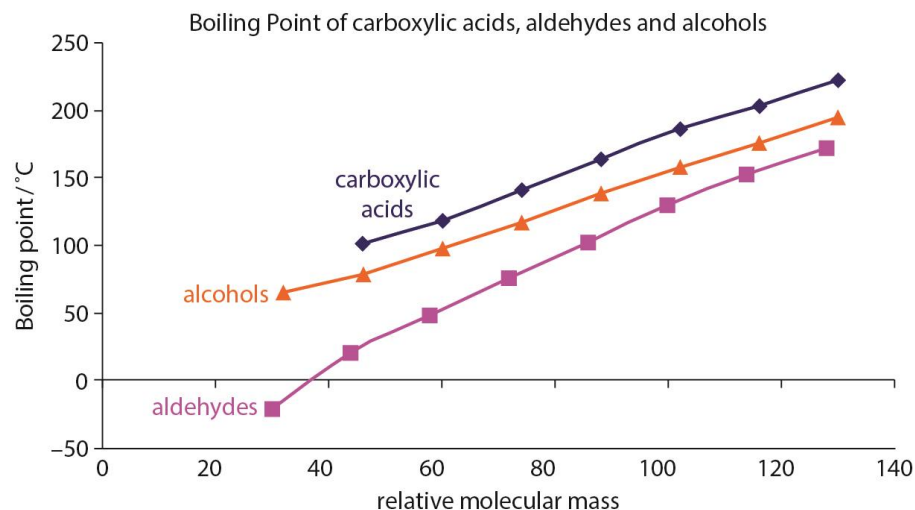


Figure 11.13: Trend in boiling points of alkanes, aldehydes and alcohols.

> Naming esters

Ester functional group

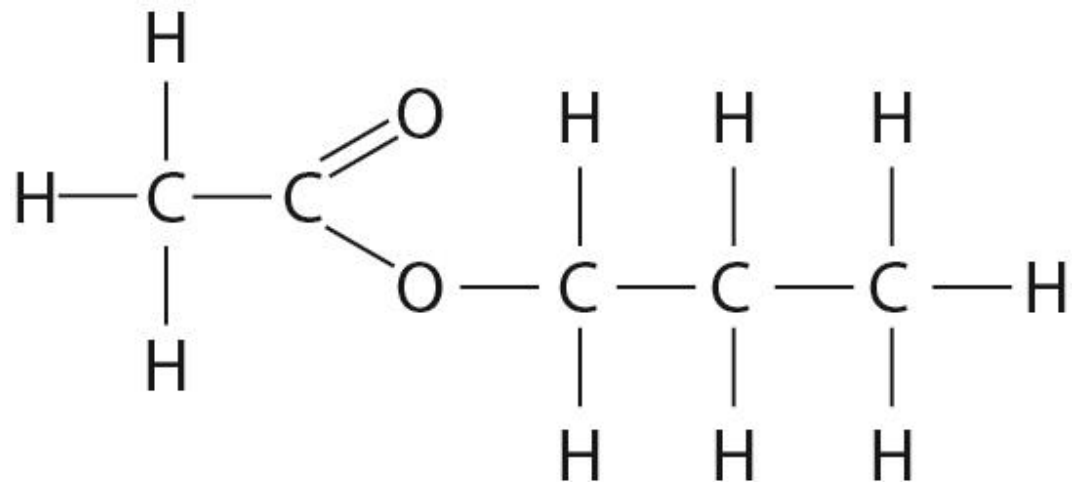
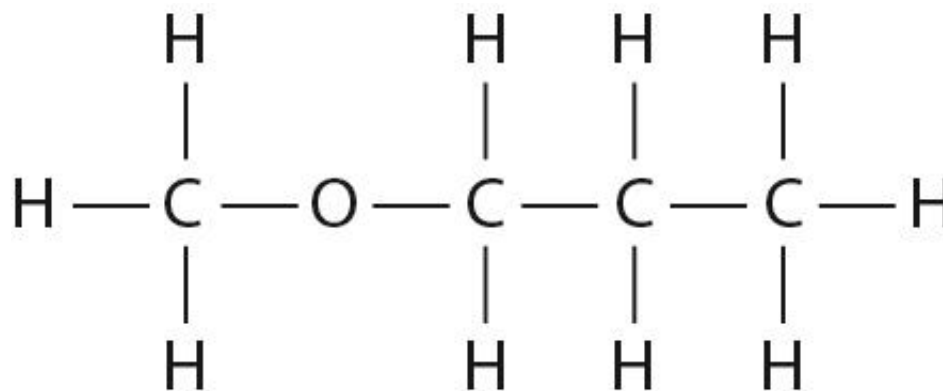


Figure 11.14: Propyl ethanoate.

> Alkoxy functional group

Ethers

a



b

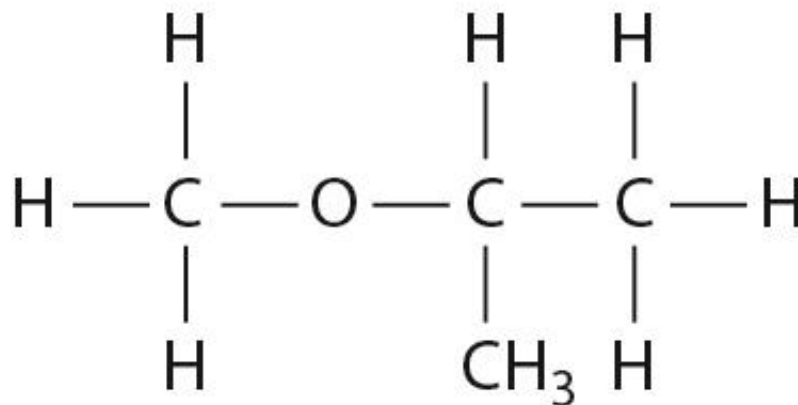


Figure 11.15: **a** 1-methoxypropane and **b** 2-methoxypropane.

> Halogenoalkanes

Halogeno functional group

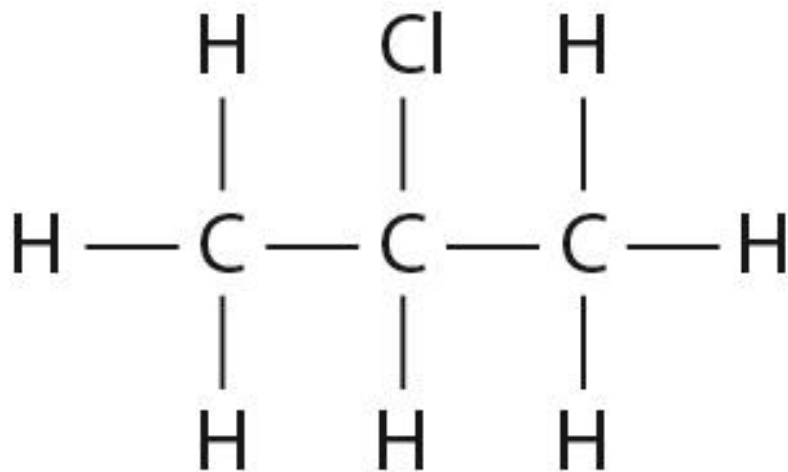


Figure 11.16: 2-chloropropane.

> Primary, secondary and tertiary

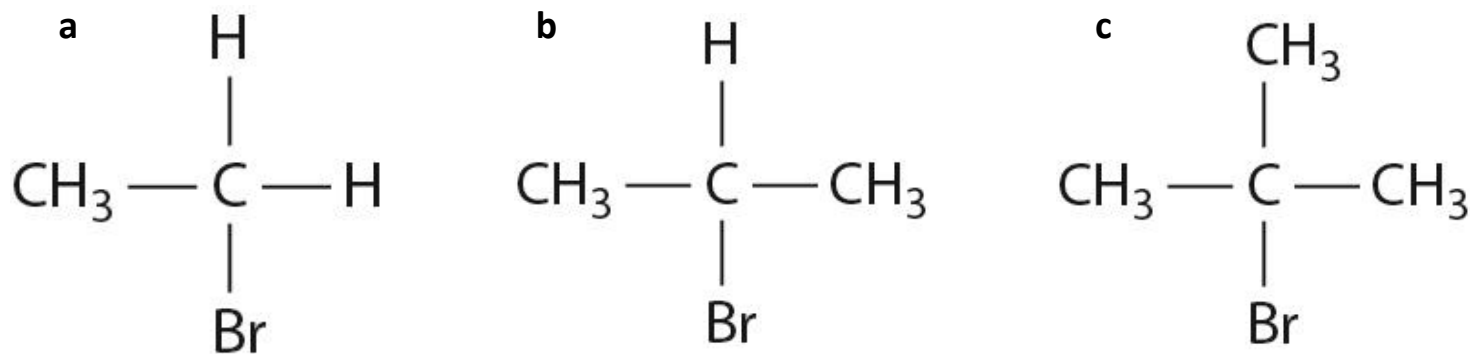


Figure 11.17: **a** Primary, **b** secondary and **c** tertiary bromoalkanes.

> Types of compounds

Aromatic compounds are compounds that contain a phenyl group.

Aliphatic compounds are compounds without phenyl groups.

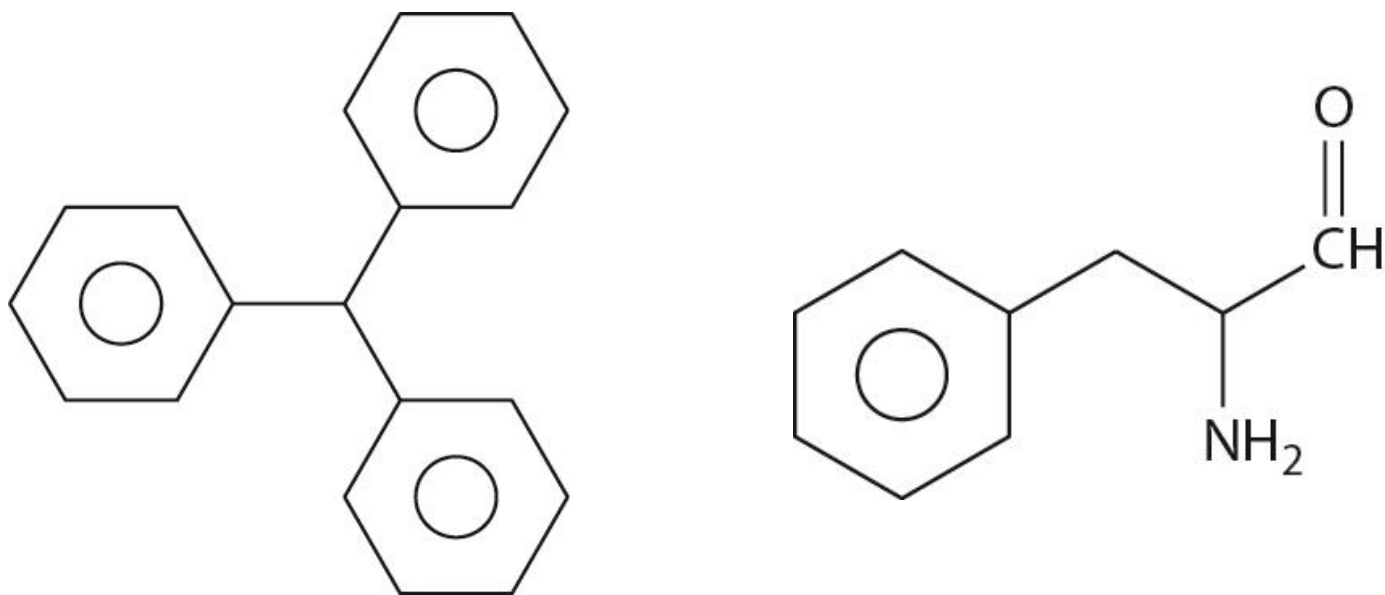


Figure 11.18: Examples of aromatic compounds.

> Evidence for the delocalised structure in benzene

Kekulé's structure of benzene

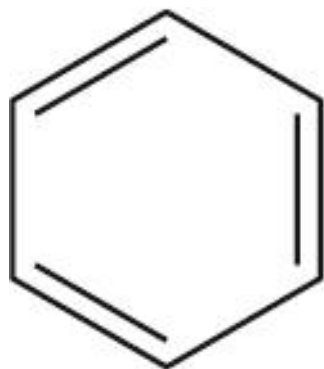


Figure 11.19: Portrait of August Kekulé.

Bond	Compound	Bond length /nm
C=C	ethene	0.133
C—C	ethane	0.154
C—C	benzene	0.140

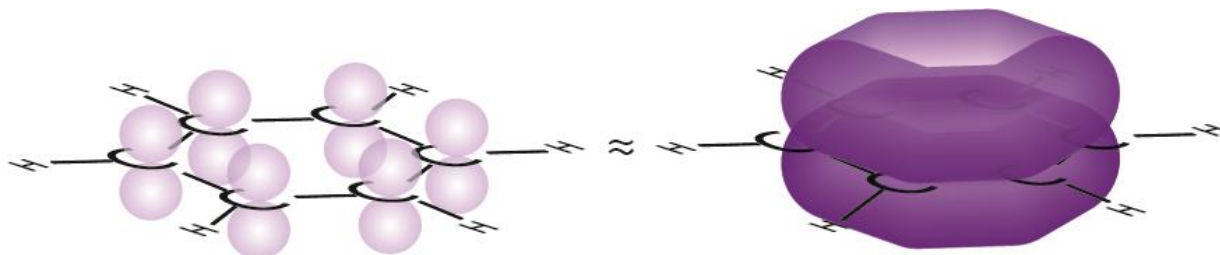


Figure 11.20: Formation of the benzene delocalised system.

> Amines

Amino functional group

	Primary	Secondary	Tertiary
Functional group	—NH_2	$\begin{array}{c} \text{—N—H} \\ \\ \text{R} \end{array}$	$\begin{array}{c} \text{—N—R} \\ \\ \text{R} \end{array}$

> Amides

Amido functional group

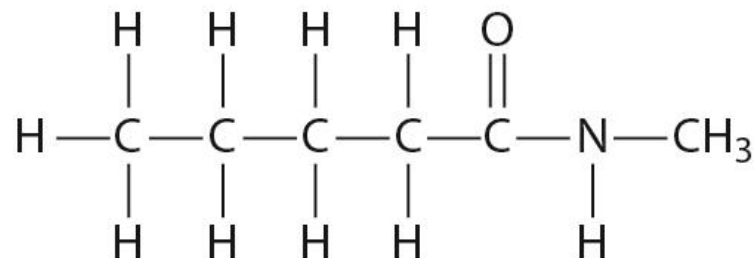
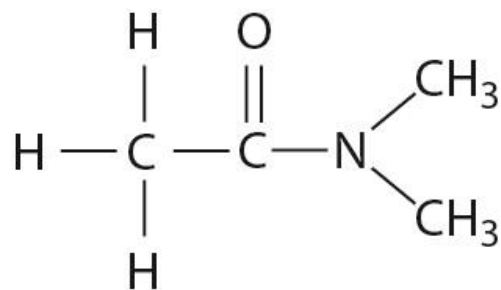
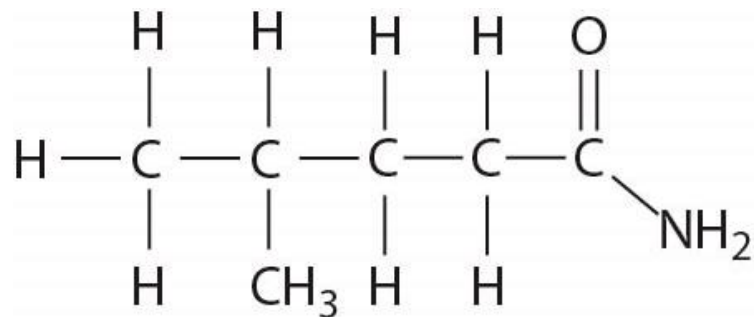
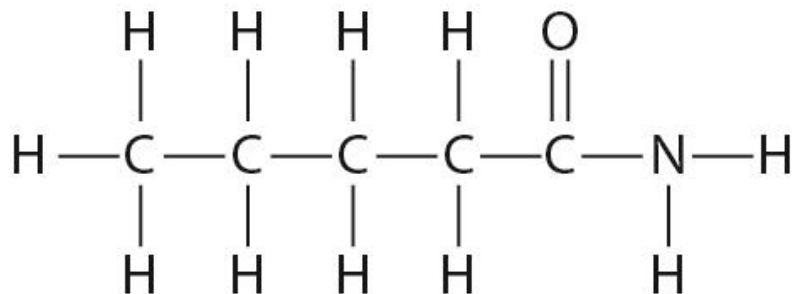
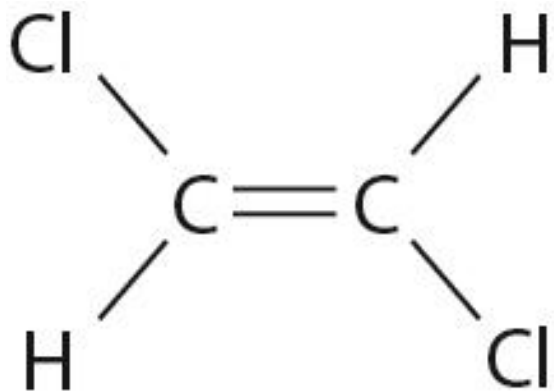


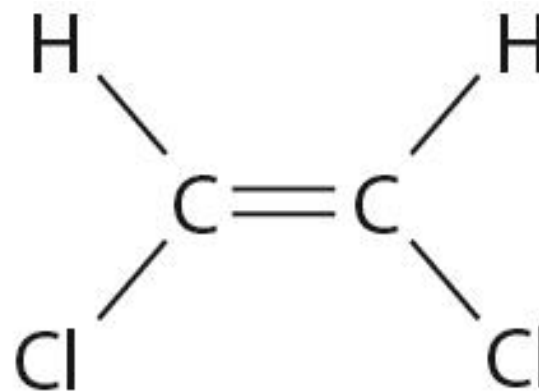
Figure 11.21: Differently substituted amides.

> *cis-trans* isomerism

Stereoisomerism



trans-1,2-dichloroethene

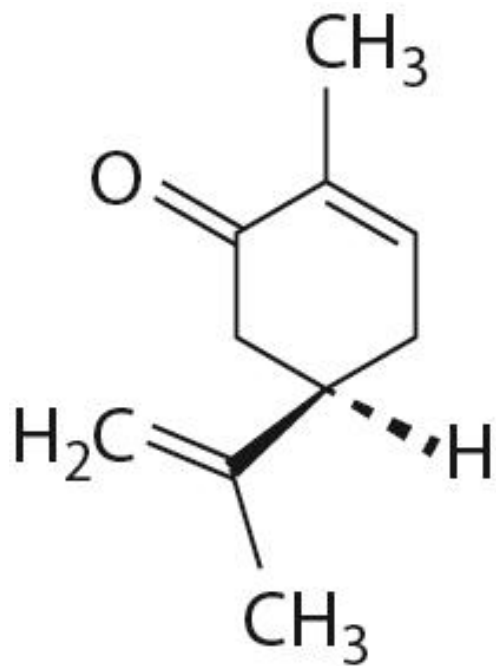


cis-1,2-dichloroethene

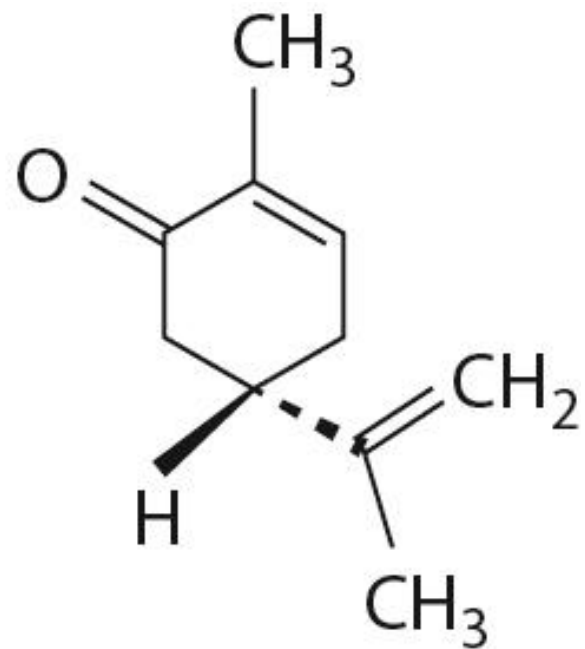
Figure 11.22: Isomers of 1,2-dichloroethene.

> Optical isomerism

Stereoisomerism



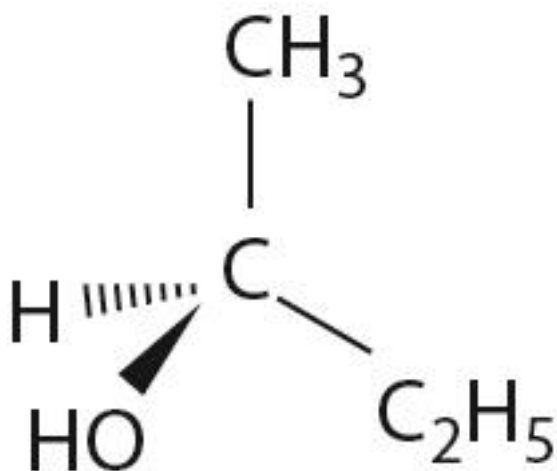
mint



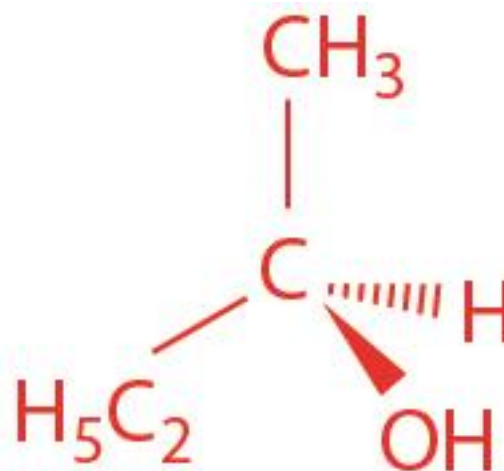
caraway

Figure 11.23: Two of the stereoisomers of carvone.

> Types of molecules



Chirality centre (chiral centre): a carbon atom with four different atoms or groups attached to it (sometimes called an asymmetric carbon atom) that makes a molecule chiral.



Enantiomers: the non-superimposable mirror images of a chiral molecule.

➤ Using a polarimeter to determine the direction in which light is rotated

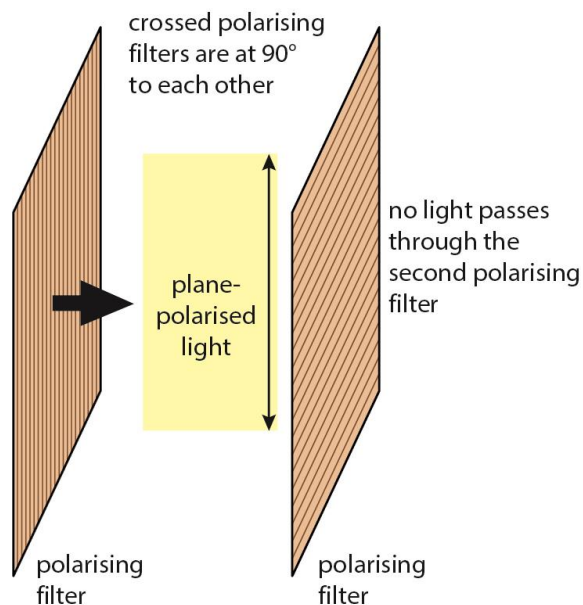


Figure 11.24: When polarising filters are crossed, no light can pass through, unless it has been rotated by an optically active sample between the first and second filters.

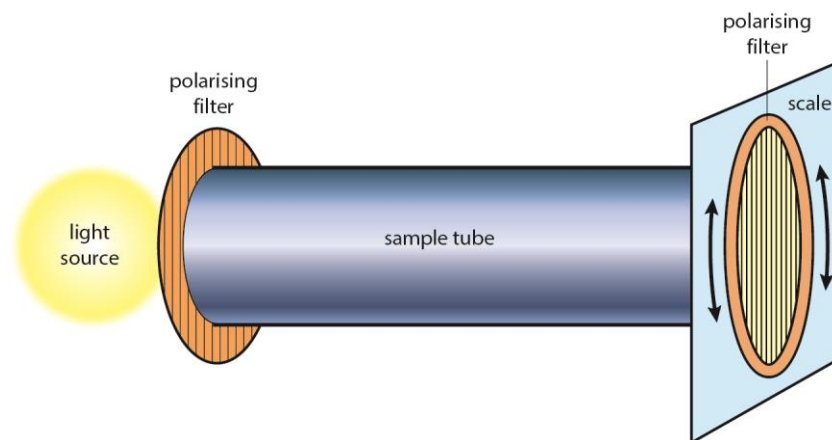


Figure 11.25: A simple polarimeter.

➤ Isomers of propanol can be identified using the fingerprint region of the IR spectra

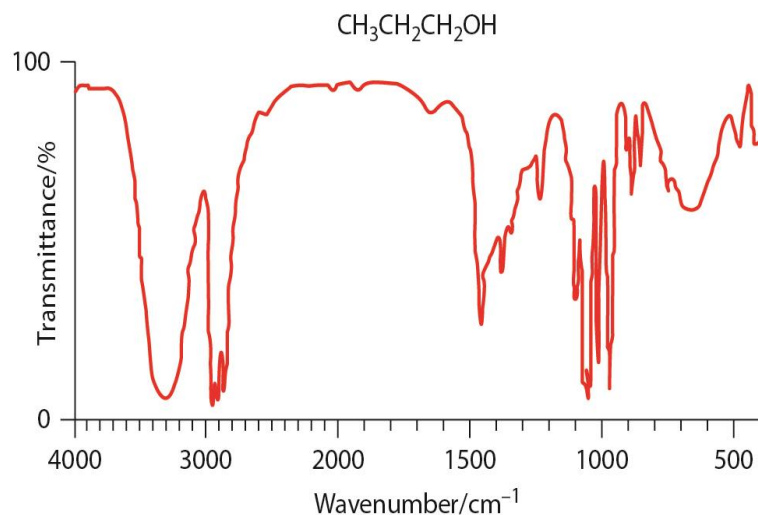


Figure 11.26: Infrared spectrum of propan-1-ol.

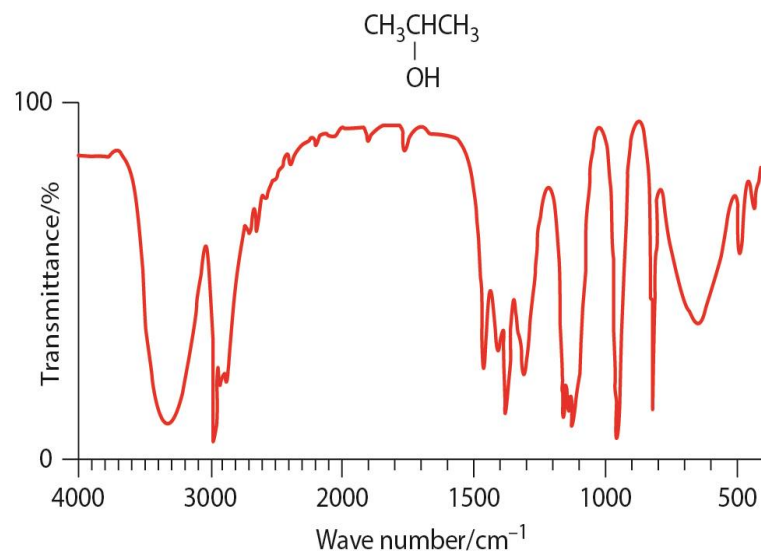
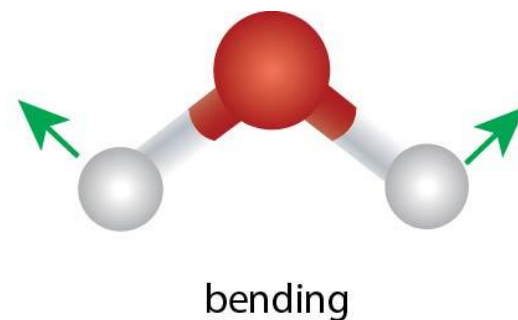
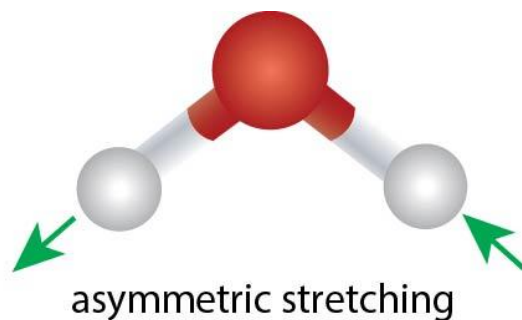
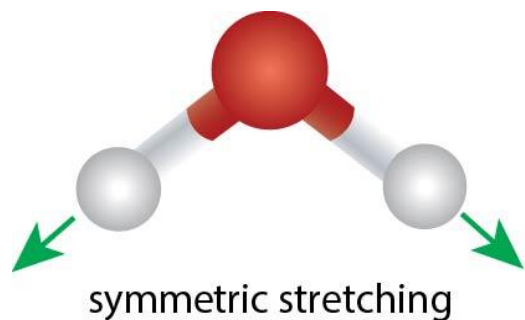


Figure 11.27: Infrared spectrum of propan-2-ol.

> Different vibrational modes of water molecules



Video 11.1: Vibrational modes of water molecules.

> Mass spectrometry

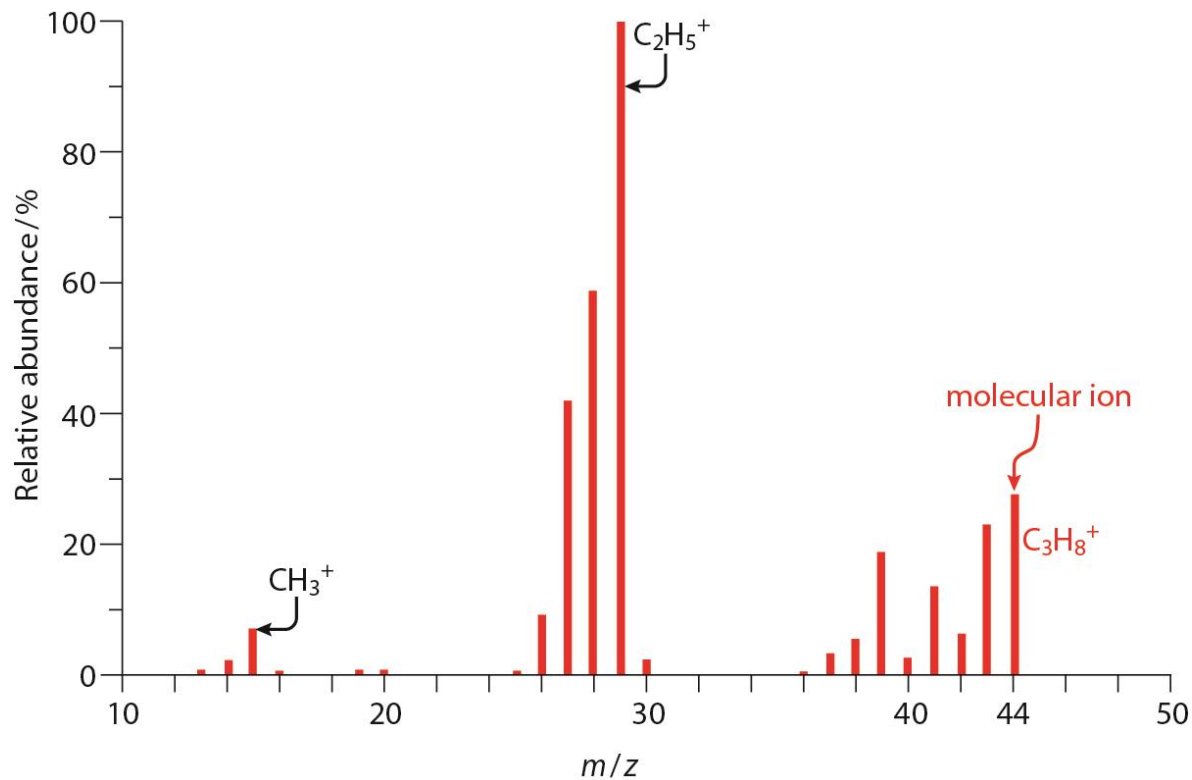


Figure 11.28: The mass spectrum of propane: $\text{CH}_3\text{CH}_2\text{CH}_3$.

> ^1H nuclear magnetic resonance (NMR)

Looking at H atoms in a molecule

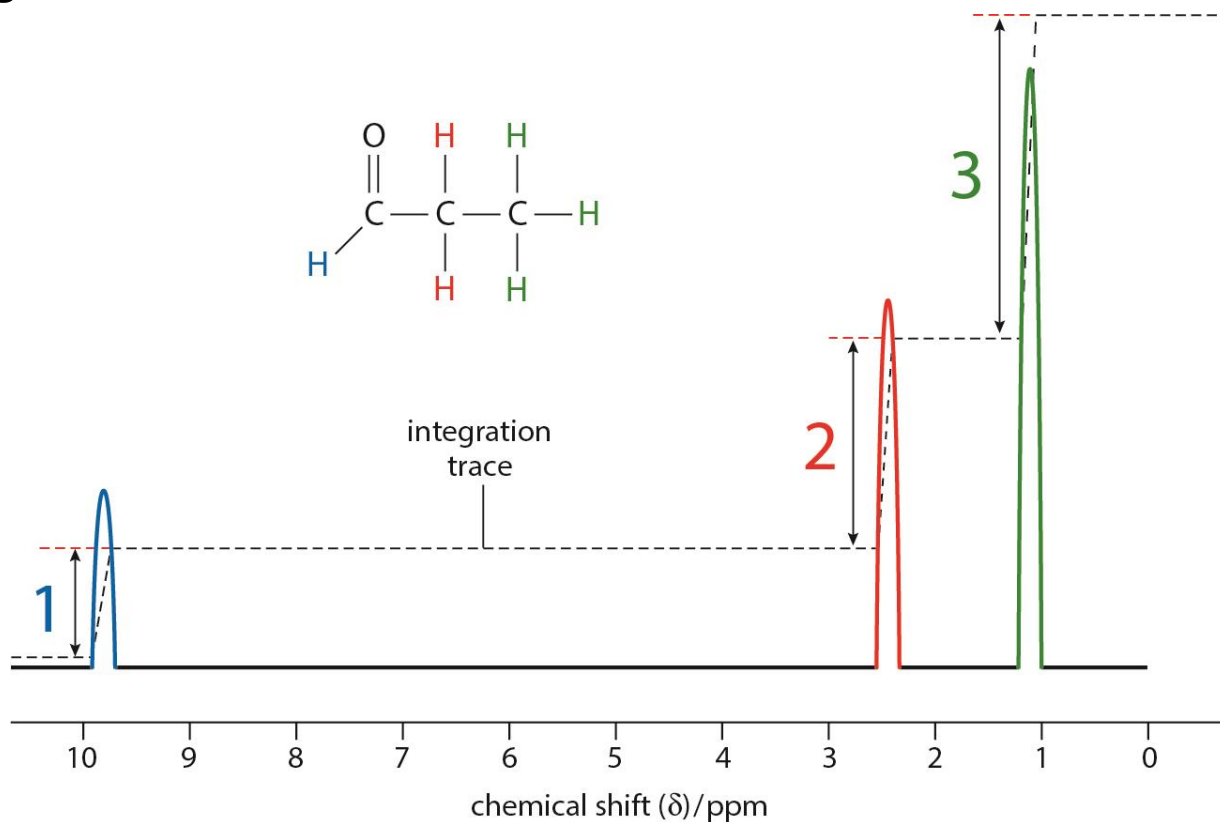


Figure 11.29: The low-resolution NMR spectrum of propanal: $\text{CH}_3\text{CH}_2\text{CHO}$. The integration trace allows us to work out the ratio of the numbers of protons in each environment.

> High-resolution NMR spectrum

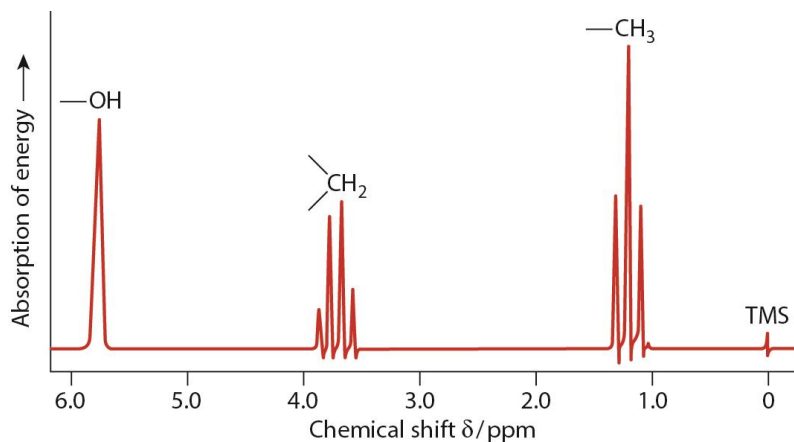


Figure 11.30: High-resolution NMR spectrum of ethanol.

No. of equivalent protons on adjacent C atoms	Pattern	Diagram
1	1:1 doublet	
2	1:2:1 triplet	
3	1:3:3:1 quartet	