

At the end of this chapter, you will appreciate the significance of the compounds that are formed between carbon, hydrogen and other elements such as oxygen and nitrogen. Carbon is only the eleventh most abundant element in the universe, yet it forms more compounds than all other elements except hydrogen.

The prevalence of carbon in living things is why the study of the compounds of carbon and hydrogen is known as organic chemistry. You make use of these compounds in so many aspects of your life: from the polymer case of your phone to the pasta that you may eat for dinner.

In this chapter, you will start to explore some of the many families of carbon compounds. You will investigate the properties of these compounds and how they are named and identified.

Science understanding

- organic molecules have a hydrocarbon skeleton and can contain functional groups, including alkenes, alcohols, aldehydes, ketones, carboxylic acids, esters, amines and amides; functional groups are groups of atoms or bonds within molecules which are responsible for the molecule's characteristic chemical properties
- structural formulae (condensed or showing bonds) can be used to show the arrangement of atoms and bonding in organic molecules that contain the following functional groups: alkenes, alcohols, aldehydes, ketones, carboxylic acids, esters, amines and amides
- IUPAC nomenclature is used to name organic species, including those with a parent chain of up to 8 carbon atoms with simple branching and one of the following functional groups: alkenes, alcohols, aldehydes, ketones, carboxylic acids, esters, amines and amides
- isomers are compounds with the same molecular formulae but different structures; different types of isomerism include chain and position structural isomerism and *cis-trans* isomerism
- organic compounds display characteristic physical properties, including boiling point and solubility in water and organic solvents; these properties can be explained in terms of intermolecular forces (dispersion forces, dipole-dipole interactions and hydrogen bonds) which are influenced by the nature of the functional groups
- empirical and molecular formulae can be determined by calculation and the structure of an organic compound established from the chemical reactions they undergo, and other analytical data

13.1 Diversity of carbon compounds

Carbon forms more compounds than all other elements combined. This is because:

- carbon has four valence electrons so carbon can potentially form covalent bonds with four other atoms
- carbon atoms can form strong covalent bonds with other carbon atoms, partly due to the relatively small size of the carbon atom
- covalent bonds formed by carbon atoms can be single, double or triple bonds.

Because of this, carbon can bond to itself to form molecules of varied length and shape. The different structures have different properties and applications.

Carbon-based molecules are all around you. Caffeine, petrol, pesticides, plastics and artificial flavours are all carbon-based compounds. Many of these compounds are produced from **crude oil**. Crude oil is formed over millions of years by the effects of heat and pressure on dead animals, plants and microorganisms trapped in the Earth's crust, buried beneath sediment. The study of the chemistry of carbon compounds is known as organic chemistry.

HYDROCARBONS

The simplest organic molecules are the **hydrocarbons**. Although hydrocarbons only contain the elements carbon and hydrogen, the different ways their atoms can be arranged to form molecules results in an enormous diversity of compounds. As you learnt in Year 11, hydrocarbon families can be simplified by grouping the millions of different molecules that exist into families called **homologous series**.

Compounds that are members of the same homologous series have:

- similar structures
- similar chemical properties
- the same general formula
- a pattern to their physical properties.

Homologous series contain members that have increasingly longer chains. The chains grow by the addition of a $-\text{CH}_2-$ unit to the previous member of the series. The hydrocarbons consist of three homologous series: the alkanes, the alkenes and the alkynes. Alkynes are not covered in this course and will not be discussed in detail.

The concept of homologous series can be applied to other types of organic molecules encountered later in this chapter.

i Alkanes and alkenes are the most common hydrocarbon homologous series. The chains grow by the addition of a $-\text{CH}_2-$ unit.

ALKANES

Hydrocarbons can be classified into several groups or series. Methane is the first of a series of compounds known as the **alkanes**. Alkanes are hydrocarbons that contain only single bonds. All the carbon-carbon bonds in alkanes are single covalent bonds. Molecules such as this are said to be **saturated**.

Each member of the alkane series differs from the previous member by a $-\text{CH}_2-$ unit. You will recall that a series of molecules in which each member differs by $-\text{CH}_2-$ from the previous member is known as a homologous series.

The diverse uses of hydrocarbons

The simplest homologous series is the alkanes. Alkanes are a homologous series of molecules that consist entirely of hydrogen and carbon atoms. Figure 13.1.1 shows methane, the simplest hydrocarbon. Methane is the gas used in most laboratory Bunsen burners. Propane (Figure 13.1.2) also belongs to the alkane homologous series. Like methane, propane is a commonly used fuel contained in many portable gas bottles. Alkenes such as ethene (Figure 13.1.3) contain a carbon-to-carbon double bond. Ethene is commonly used to make polymers that are found in many household plastics. Some hydrocarbons can also form ring structures like those shown in Figures 13.1.4 and 13.1.5. These rings may form from single carbon-to-carbon bonds or even double bonds like those shown in benzene in Figure 13.1.5.

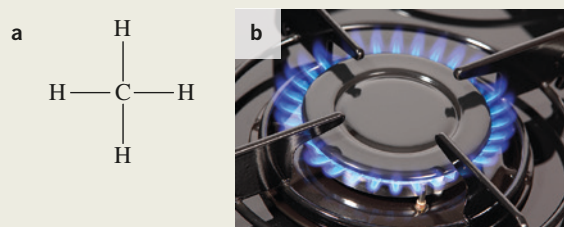


FIGURE 13.1.1 (a) Methane (CH_4) contains one carbon atom with four single covalent bonds to four hydrogen atoms. (b) Methane is the gas used in most laboratory Bunsen burners and household gas stoves.

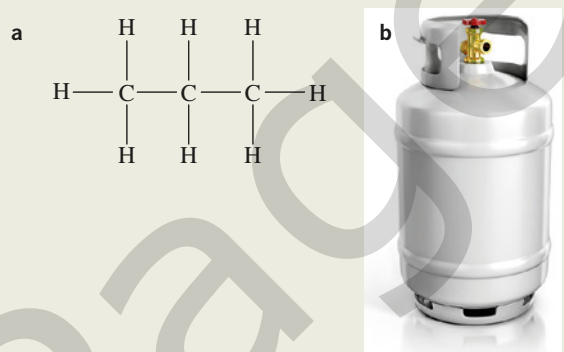


FIGURE 13.1.2 (a) Propane (C_3H_8) contains only single bonds. (b) Propane is the fuel contained in many portable gas bottles.



FIGURE 13.1.3 (a) Carbon can form compounds that contain carbon-carbon double bonds. These compounds include ethene (C_2H_4). (b) Among other uses, ethene is used to make the polymers in these food storage containers.

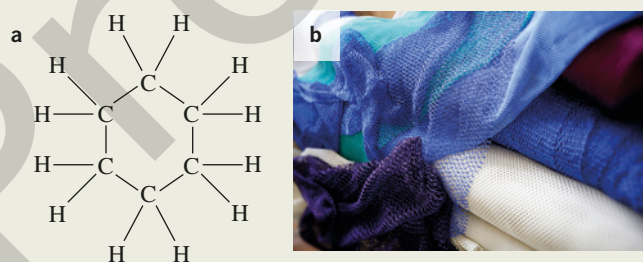


FIGURE 13.1.4 (a) Hydrocarbons can form ring structures with single bonds, such as cyclohexane (C_6H_{12}). (b) Cyclohexane is used by industry to make the starting materials for the manufacture of nylon.

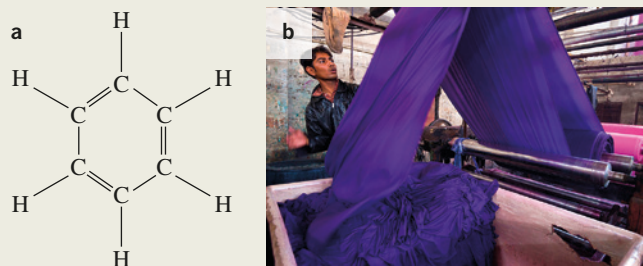
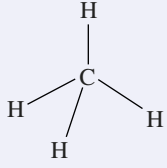
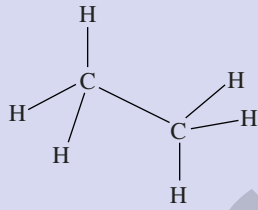
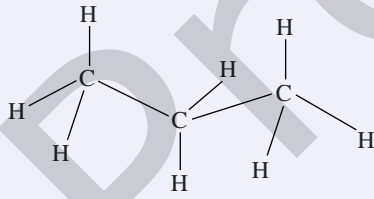


FIGURE 13.1.5 (a) Some molecules containing rings are unsaturated, such as benzene (C_6H_6), which is found in crude oil. (b) In this image, a textile is dyed using a dye based on benzene.

Table 13.1.1 shows the first three members of the alkane series. Note that the bonds around each carbon atom adopt a tetrahedral shape and the boiling points increase as the molecules become larger.

TABLE 13.1.1 Structure, properties and some uses of the first three alkanes

Name and molecular formula	Structural formula	Properties	Uses
Methane, CH ₄		Non-polar, gas, boiling point (BP) -164°C	Cooking, Bunsen burners, gas heating
Ethane, C ₂ H ₆		Non-polar, gas, BP -87°C	Conversion to ethene
Propane, C ₃ H ₈		Non-polar, gas, BP -42°C	Liquid petroleum gas (LPG)

REPRESENTING ORGANIC MOLECULES

Before exploring organic molecules further, you should revise the different ways that the formulae of molecules can be represented. The formulae used in this course are:

- molecular formulae
- structural formulae
- condensed (or semistructural) formulae.

Molecular formulae

Molecular formulae such as C₂H₆O and C₄H₈O₂ indicate the number and type of atoms of each element present in a molecule. However, they do not indicate how the atoms are arranged.

Structural formulae

Structural formulae show the spatial location of atoms relative to one another in a molecule, as well as the number and location of covalent bonds. Non-bonding electrons (lone pairs) are generally not shown.

As you learnt in Year 11, when four single bonds are formed around a carbon atom, the pairs of electrons in each bond act as a negatively charged cloud. **Valence shell electron pair repulsion (VSEPR) theory** tells you that these electron pairs repel each other so the bonds are as far apart as possible, at an angle to each other of nearly 109.5°. The structure of methane, shown in Figure 13.1.6, is described as a **tetrahedral** shape because the four single bonds are pointing to the corners of a tetrahedron (shown in red).

Molecules consisting of long chains of carbon atoms joined by single bonds are often referred to as 'straight-chain' molecules. However, because of the tetrahedral distribution of each carbon's bonds, the chain actually has a zig-zag shape. Structural formulae showing a tetrahedral arrangement of bonds can become

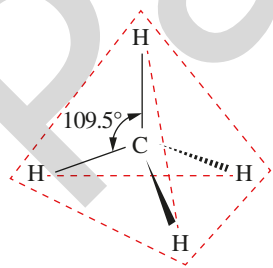


FIGURE 13.1.6 The structure of a molecule of methane (CH₄) showing the tetrahedral geometry. The solid wedge represents a bond coming out of the page, whereas the dashed wedge represents a bond going into the page.

complicated and difficult to interpret. To make the structure of these molecules clearer, the bonds are often drawn at right angles. These two representations are shown in Figure 13.1.7.

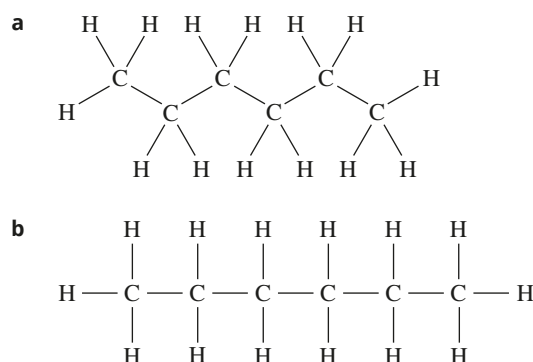


FIGURE 13.1.7 (a) The six carbon chain of hexane (C_6H_{14}). There is a tetrahedral arrangement of bonds around each carbon atom. (b) The chain can be drawn in a straight line for convenience.

Condensed formulae

A **condensed formula** is used to indicate the connections in the structure of a compound without showing the three-dimensional arrangement of atoms. The term **semistructural formula** is also used to describe this type of formula.

In a condensed formula, the carbon chain is represented on one line of text. The carbon atoms in the chain, and all the atoms attached to each of them, are listed in the order that they appear in the structural formula. Single bonds are not shown but double carbon-carbon bonds are often shown. Groups of atoms that form branches in a molecule are written in brackets after the carbon atom to which they are attached. Some examples of structural, condensed and molecular formulae are shown in Table 13.1.2.

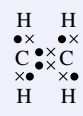
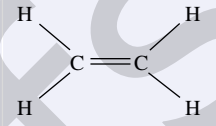
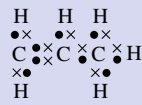
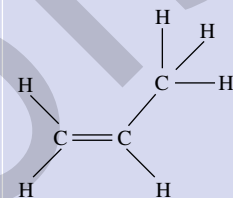
TABLE 13.1.2 Examples of structural, condensed and molecular formulae

Structural formula and name	Condensed (semistructural) formula	Molecular formula
<p>Butane</p>	$CH_3CH_2CH_2CH_3$	C_4H_{10}
<p>But-1-ene</p>	$CH_2=CHCH_2CH_3$	C_4H_8
<p>2-Methylbutan-1-amine</p>	$CH_3CH_2CH(CH_3)CH_2NH_2$	$C_5H_{13}N$

Writing formulae of alkenes

As with alkanes, there are a variety of ways for writing the formulae of alkenes. Table 13.1.3 shows different ways of representing ethene and propene.

TABLE 13.1.3 Different ways of representing alkenes

Alkene	Molecular formula	Electron dot diagram (Lewis structure)	Condensed structural formula	Structural formula
Ethene	C ₂ H ₄		CH ₂ CH ₂	
Propene	C ₃ H ₆		CH ₂ CHCH ₃	

NAMING ORGANIC MOLECULES

As you learnt in Year 11, the IUPAC (International Union of Pure and Applied Chemists) system is used to name organic molecules. In Year 12, you will be using this system to name a range of molecules, including **isomers**, from different homologous series of organic substances. The following section revises some of the naming techniques that you used in Year 11.

The **stem names** used for molecules with between one and eight carbon atoms are listed in Table 13.1.4.

TABLE 13.1.4 Stem names used for molecules with between one and eight carbon atoms

Stem (parent) name	Number of carbon atoms
meth-	1
eth-	2
prop-	3
but-	4
pent-	5
hex-	6
hept-	7
oct-	8

Naming alkanes

The systematic naming of carbon compounds is controlled by IUPAC. Under the IUPAC system, the name of the compound provides details of its structure. The following rules apply when naming alkanes.

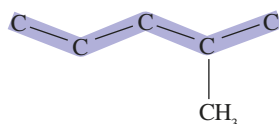
1. Identify the longest unbranched carbon chain.
2. Number the carbon atoms in the chain from the end of the chain that will give the smallest numbers to branching groups.
3. Name the alkyl groups after the alkane from which they are derived.
4. Place the number and position of each of the alkyl groups at the beginning of the compound's name.
5. If two identical side chains are present, use 'di-' as a prefix; for three, use 'tri-'.

6. If there are more than one type of alkyl side chains on the molecule, list them in alphabetical order at the start of the name, with their numbers to indicate their respective positions.

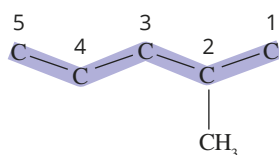
i Carefully check that you have identified the longest unbranched carbon chain. Sometimes the longest carbon chain is not drawn in a straight line.

The following steps show the process of naming the isomer of hexane shown in Figure 13.1.8.

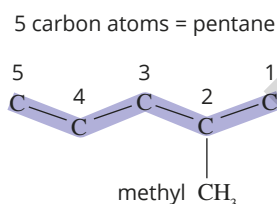
1. Identify the longest unbranched carbon chain.



2. Number the carbons, starting from the end closest to the branch.



3. Name the side branches and main chain.



4. Combine all components to write the full name: 2-methylpentane

Figure 13.1.9 shows examples of applications of these rules. Note the use of the prefix 'di-' to indicate the presence of two methyl side branches and the numbering to indicate their position along the longest continuous carbon chain (for example, 3,3-indicates that both side branches are attached to the third carbon atom).

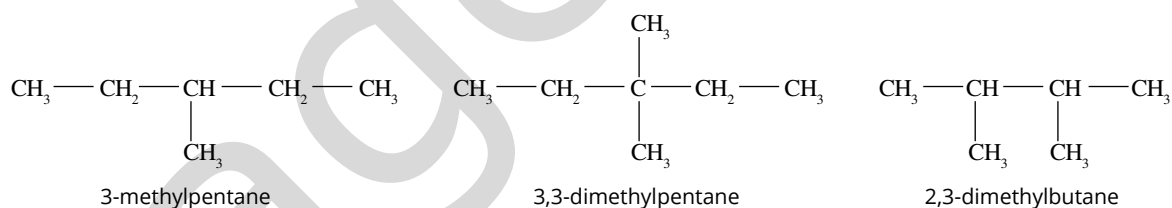


FIGURE 13.1.9 IUPAC systematic names for three alkanes. Note that there are no spaces in the names of these compounds.

ALKENES

Alkenes are unsaturated hydrocarbons and contain at least one double carbon-carbon bond, so must contain two or more carbon atoms.

The homologous series of hydrocarbons that contains a carbon-carbon double bond is called the alkenes. The molecular, structural and condensed formulae of the first three members of the homologous series of alkenes are shown in Table 13.1.5. You can see that successive members differ by a $-\text{CH}_2-$ unit. Alkenes have the general formula C_nH_{2n} .

Alkenes with four or more carbon atoms can have **structural isomers**, where the location of the double bond changes, as well as **cis-trans isomers**, where the geometry of groups around the double bond changes.

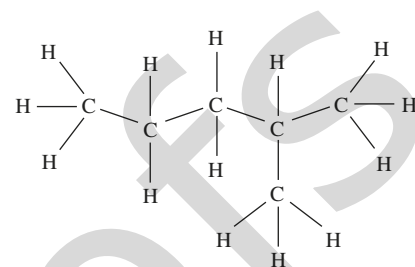
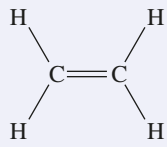
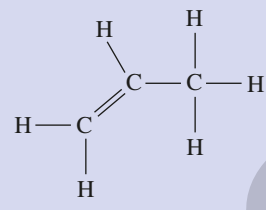
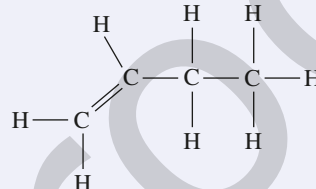


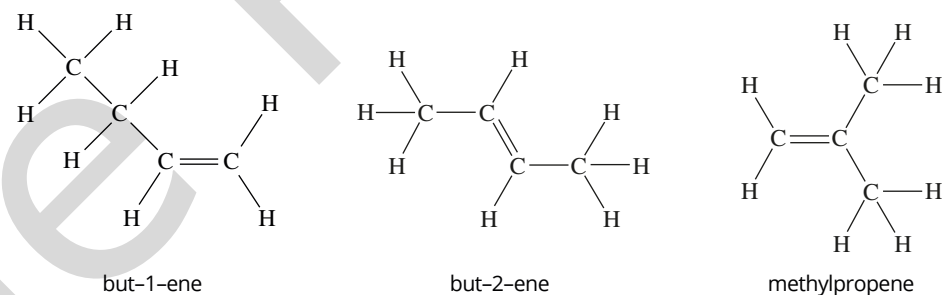
FIGURE 13.1.8 The IUPAC system will be used to name this isomer of hexane.

TABLE 13.1.5 Formulae of the first three members of the alkene homologous series

Name	Molecular formula	Structural formula	Condensed structural formula
Ethene	C ₂ H ₄		CH ₂ =CH ₂
Propene	C ₃ H ₆		CH ₂ =CHCH ₃
But-1-ene	C ₄ H ₈		CH ₂ =CHCH ₂ CH ₃

Structural isomers of alkenes

For alkene molecules that contain more than three carbon atoms, structural isomers will exist. As you can see in Figure 13.1.10, isomers may result from branches in the carbon chain, or if the carbon–carbon double bond is in different positions.

**FIGURE 13.1.10** Isomers of butene. Isomers of alkenes can have branches in the carbon chain or the double bond at different points in the carbon chain.

When naming alkene isomers, the carbons are numbered from the end of the carbon chain that gives the lowest number to the first carbon in the double bond. The location of the double bond in the molecule is indicated by this number. In Figure 13.1.10, you can see that the double bond in but-1-ene is between carbons 1 and 2. The double bond in but-2-ene is between carbons 2 and 3.

Naming alkenes

The rules for naming alkenes follow the rules used for alkanes. In addition, the following conventions are applied.

- Use the ending ‘-ene’ for the parent name.
- Number the carbon atoms from the end of the chain closest to the double bond.
- Specify the position of the double bond by the number of the lowest-numbered carbon atom in the double bond.
- Insert the number into the name immediately before ‘-ene’.
- Indicate *cis* and *trans* isomers by writing ‘*cis*-’ or ‘*trans*-’ in front of the compound’s name.

The flowchart in Figure 13.1.11 shows the steps involved in naming an alkene.

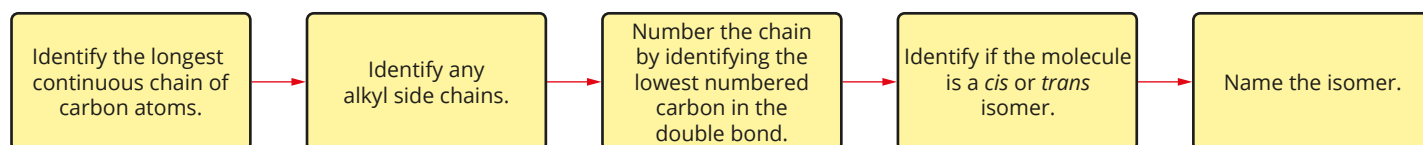


FIGURE 13.1.11 The steps used to name alkenes

Worked example 13.1.1

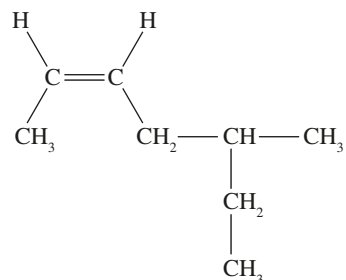
NAMING A *cis-trans* ISOMER OF AN ALKENE

Write the systematic name of the following alkene.	
Thinking	Working
Identify the parent name by counting the longest continuous chain of carbon atoms that contains the carbon-carbon double bond.	<p>There are five carbon atoms in the longest continuous chain, so the parent name is pentene.</p>
Identify any alkyl side chains by counting the number of carbon atoms in any branches.	There are no alkyl side chains.
Number the continuous chain from the end closest to the double bond and identify the lowest numbered carbon atom in the double bond.	<p>The lowest numbered carbon atom in the double bond is 2, so the parent name becomes pent-2-ene.</p>
Number any alkyl side chains using the numbers of the carbon atoms to which they are attached.	There are no alkyl side chains.
Identify whether the molecule is a <i>cis</i> or <i>trans</i> isomer.	<p>Both of the carbons in the double bond are attached to a hydrogen atom and another carbon in the chain. The carbon atoms are on opposite sides of the double bond so this is a <i>trans</i> isomer.</p>
Name the isomer.	The name of the isomer is <i>trans</i> -pent-2-ene.

Worked example: Try yourself 13.1.1

NAMING A *cis-trans* ISOMER OF AN ALKENE

Write the systematic name of the following alkene.



BENZENE RINGS

In 1825, Michael Faraday isolated a new hydrocarbon, named benzene (C₆H₆). The structure and properties of benzene puzzled scientists for 40 years. It is now known that benzene has a ring structure, but it does not have alternating double and single bonds (Figure 13.1.12).

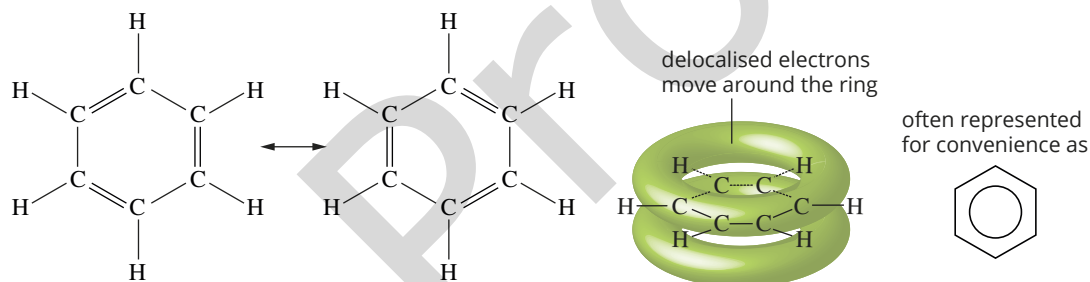


FIGURE 13.1.12 Representations of benzene. All six carbon atoms and six hydrogen atoms in the benzene molecule are in the same plane. There are no double bonds in benzene: the electrons are delocalised.

The electrons that make up the double bonds are not in fixed positions; they are delocalised and can move around the ring. Each carbon-carbon bond is the same length and the molecule is more stable than you would expect an unsaturated molecule to be.

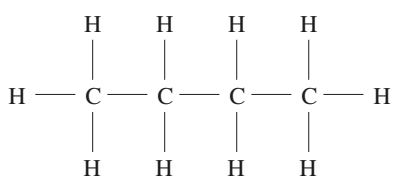
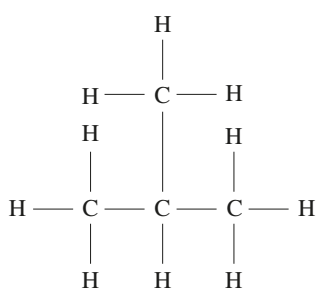
In Year 11, you saw that benzene is a substance that can exist on its own. Benzene rings can also exist within more complex molecules, or as a side group on a molecule. In this context, the benzene ring is called a phenyl group, and later in this chapter you will encounter substances, such as phenylamine (used as an artificial sweetener in drinks) that contain benzene rings.

13.1 Review

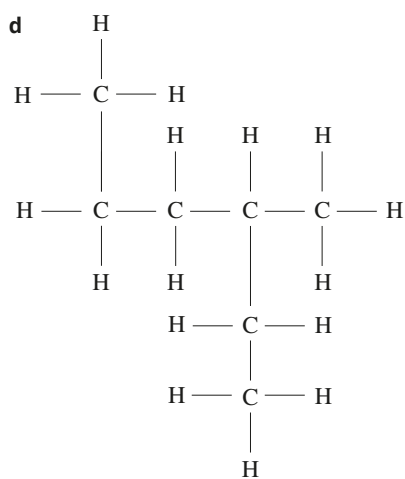
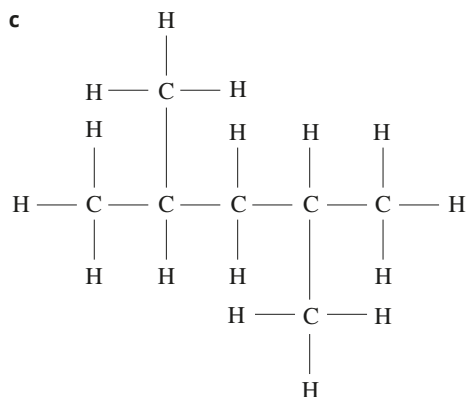
SUMMARY

- Hydrocarbons are compounds containing carbon and hydrogen only.
- In a homologous series, each member has one more $-\text{CH}_2-$ unit than the previous member. Members of a homologous series have similar structures and chemical properties and the same general formula. Alkanes are an example of a homologous series.
- Alkanes are saturated hydrocarbon molecules that contain only single bonds and have a general formula $\text{C}_n\text{H}_{2n+2}$.
- Structural isomers are molecules with the same molecular formula but different arrangements of atoms.
- Hydrocarbon molecules can be drawn using structural formulae or condensed structural formulae.
- The IUPAC naming system is used to provide systematic names for hydrocarbon molecules. Names are based on the longest unbranched carbon chain.
- Alkenes are a homologous series of hydrocarbons that contain a carbon-carbon double bond.
- Alkenes have the general formula C_nH_{2n} .
- Alkenes can have both structural and *cis-trans* isomers.

KEY QUESTIONS

- From which one or more of the following sources does crude oil originate?
 - Plant material
 - Forest animals that have recently died
 - Dinosaurs only
 - Marine microorganisms
- Methane is the smallest hydrocarbon molecule.
 - What is the molecular formula of methane?
 - Why is methane a hydrocarbon?
 - Why does the carbon atom in a methane molecule bond to four, rather than two, three, five or any other number of hydrogen atoms?
 - Draw the structural formula of methane. Why does methane have this particular arrangement of hydrogen atoms around each carbon atom?
- Answer the following questions relating to the hydrocarbon with the molecular formula C_3H_8 .
 - What is the name of this hydrocarbon?
 - Write a balanced chemical equation for the complete combustion of this hydrocarbon. This hydrocarbon exists as a gas at room temperature.
 - Draw the structural formula of this hydrocarbon.
 - Write the condensed structural formula of this hydrocarbon.
- Write the systematic names of these alkanes based on their condensed structural formulae.
 - $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$
 - $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$
 - $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$
 - $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$
 - $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}_3)_2$
- Write the systematic names of the alkanes shown here based on their structural formulae.
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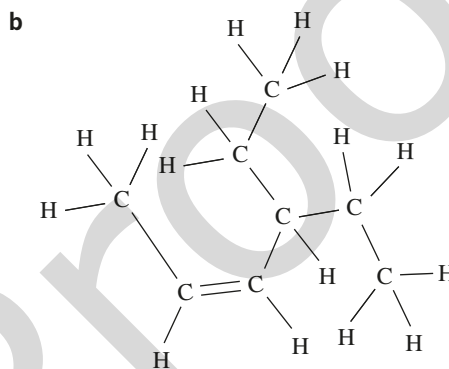
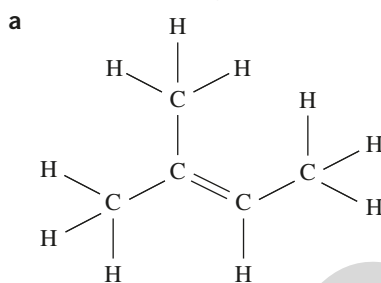
13.1 Review *continued*



6 Draw the structural formulae of these alkanes based on their systematic names.

- a** Hexane
- b** 3-Methylhexane
- c** 3,3-Dimethylpentane
- d** 3-Ethyl-2-methylpentane

7 Name the following molecules.



8 Draw the structure of 2,3-dimethylpent-2-ene.

13.2 Functional groups

Most organic compounds can be regarded as derivatives of hydrocarbons that have one or more hydrogen atoms replaced by other atoms or groups of atoms called a **functional group**.

The presence of a particular functional group in a molecule gives a substance certain physical and chemical properties. For example, vinegar and wine (Figure 13.2.1) both contain organic molecules based on ethane. The difference between their tastes and other properties is due to the different functional groups in each molecule.



FIGURE 13.2.1 (a) Vinegar and (b) wine contain molecules with two carbon atoms. Vinegar contains ethanoic (acetic) acid with a carboxyl functional group and wine contains ethanol with a hydroxyl group.

In this section, you will explore these homologous series:

- alcohols
- primary amines
- carboxylic acids
- amides
- esters
- aldehydes
- ketones.

You will learn about the functional groups in each of these families of molecules as well as how to name them.

ALCOHOLS

Ethanol is a member of the homologous series of alcohols. **Alcohols** contain a **hydroxyl** ($-\text{OH}$) **functional group** attached to a saturated carbon atom. A representation of the hydroxyl group is shown in Figure 13.2.2.

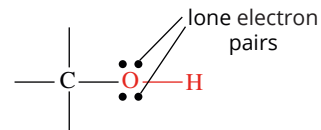


FIGURE 13.2.2 Alcohols contain the hydroxyl functional group, $-\text{OH}$ (in red above). There are two pairs of non-bonding electrons on the oxygen atom.

Figure 13.2.3 shows the structural and condensed formulae of three alcohols. You can think of the hydroxyl group as taking the place of a hydrogen atom in an alkane.

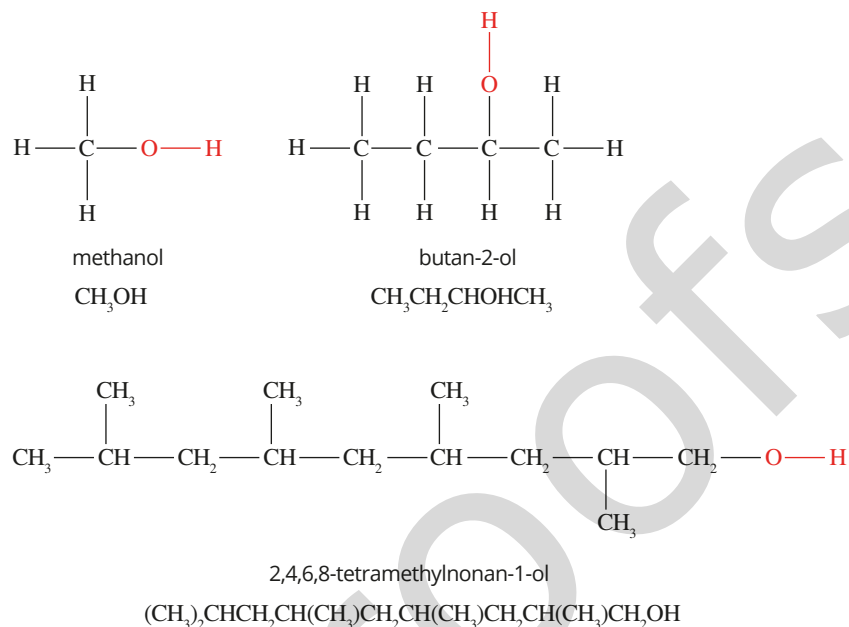


FIGURE 13.2.3 Structural and condensed formulae of three alcohols. Each contains the hydroxyl functional group (shown in red). Note that the non-bonding electron pairs on the oxygen atom are often omitted in structural formulae.

Formulae and structure of alcohols

The functional group in alcohols is made up of an oxygen atom bonded to a hydrogen atom. This $-\text{OH}$ group is known as a hydroxyl group and replaces one hydrogen in the structure of an alkane. Successive members of this homologous series differ by a $-\text{CH}_2-$ unit.

When naming alcohols, a similar systematic naming process to the one used for alkanes and alkenes applies. The number of carbon atoms in the molecule is indicated by the stem name, e.g. meth-, eth-, prop-, but-. However, the suffix (ending) of the name of an alcohol is always '-ol'. Table 13.2.1 shows different ways to represent alcohols.

TABLE 13.2.1 The first three members of the homologous series of alcohols

Alcohol	Molecular formula	Electron dot formula (Lewis structure)	Structural formula	Condensed structural formula
Methanol	CH_3OH			CH_3OH
Ethanol	$\text{C}_2\text{H}_5\text{OH}$			$\text{CH}_3\text{CH}_2\text{OH}$
Propanol	$\text{C}_3\text{H}_7\text{OH}$			$\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$

Structural isomers of alcohols

The position of the hydroxyl ($-\text{OH}$) functional group influences the chemical and physical properties of alcohols. Alcohols with more than two carbon atoms have more than one position where the hydroxyl functional group may be found. For example, the hydroxyl group in propanol ($\text{C}_3\text{H}_7\text{OH}$) can be bonded to the first or the second carbon atom. This gives two different molecules: $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ and $\text{CH}_3\text{CH}(\text{OH})\text{CH}_3$. The name of the alcohol must reflect the structure of the molecule, so a system of nomenclature is used.

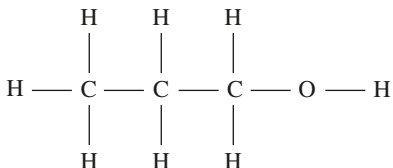
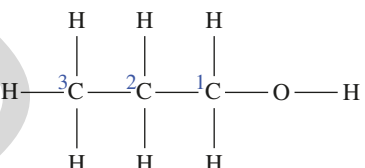
Naming alcohols

You can determine the name of an alcohol as follows.

- Start with the name of the parent alkane, remove the 'e' from the end and add the suffix '-ol'.
- Number the atoms in the longest carbon chain from the end that is closest to the $-\text{OH}$ functional group.
- Indicate the number of the atom that the hydroxyl group is bonded to before the -ol ending and separate it by hyphens.

Worked example 13.2.1

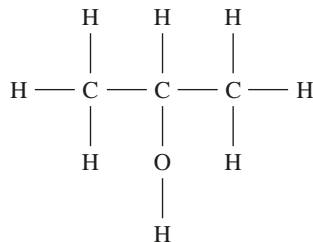
IUPAC NAMING SYSTEM FOR ALCOHOLS

Write the systematic name for the following molecule. 	
Thinking	Working
Identify the longest carbon chain in the molecule. The name of the molecule is based on this longest chain.	There are 3 carbons in the longest chain. The name is based on propane.
Identify the functional group that is present.	There is a hydroxyl group present.
Number the carbon atoms, starting from the end closest to the functional group.	
Identify the position(s) and type(s) of branches.	There are no branches in this molecule.
Combine all components. Place the number for the position of the branch in front of the prefix, and the number for the position of the hydroxyl group in front of the -ol ending.	The name of the molecule is propan-1-ol.

Worked example: Try yourself 13.2.1

IUPAC NAMING SYSTEM FOR ALCOHOLS

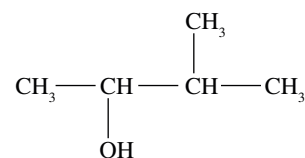
Write the systematic name for the following molecule.



Worked example 13.2.2

IUPAC NAMING SYSTEM FOR ALCOHOLS

Write the systematic name for the following molecule.



Thinking

Identify the longest carbon chain in the molecule.
The name of the molecule is based on this longest chain.

Identify the functional group that is present.

Number the carbon atoms, starting from the end closest to the functional group.

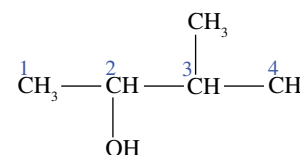
Identify the position(s) and the type(s) of branches.

Combine all components. Place the number for the position of the branch in front of the prefix, and the number for the position of the hydroxyl group in front of the -ol ending.

Working

There are 4 carbons in the longest chain.
The name is based on butane.

There is a hydroxyl group present.



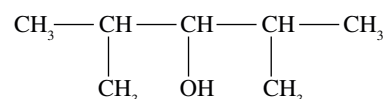
There is a methyl (-CH₃) group bonded to carbon C3 so the prefix 'methyl' is used.

The name of the molecule is 3-methylbutan-2-ol.

Worked example: Try yourself 13.2.2

IUPAC NAMING SYSTEM FOR ALCOHOLS

Write the systematic name for the following molecule.



Types of alcohols

Alcohols are classified according to the number of alkyl groups attached to the carbon atom that is bonded to the hydroxyl group. The three different types of alcohols are:

- **primary alcohols**
- **secondary alcohols**
- **tertiary alcohols.**

The definition of each type and examples are shown in Table 13.2.2. Alkyl groups are represented by the general symbol R.

TABLE 13.2.2 The three different types of alcohols. The hydroxyl group is shown in red

Type of alcohol	Definition	General formula	Example
Primary	The carbon bonded to the -OH group is only bonded to one alkyl group.	$\begin{array}{c} \text{H} \\ \\ \text{R}-\text{C}-\text{OH} \\ \\ \text{H} \end{array}$	$\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{O}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$
Secondary	The carbon bonded to the -OH group is also bonded to two alkyl groups.	$\begin{array}{c} \text{R} \\ \\ \text{H}-\text{C}-\text{OH} \\ \\ \text{R} \end{array}$	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{O}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \text{H} \quad \text{H} \end{array}$
Tertiary	The carbon atom bonded to the -OH group is also bonded to three alkyl groups.	$\begin{array}{c} \text{R} \\ \\ \text{R}-\text{C}-\text{OH} \\ \\ \text{R} \end{array}$	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \text{H} \quad \text{O} \\ \quad \quad \quad \\ \quad \quad \quad \text{H} \end{array}$

PRIMARY AMINES

Amines are a homologous series of organic compounds that contain the **amino functional group**. An amino functional group consists of one nitrogen atom covalently bonded to two hydrogen atoms as shown in Figure 13.2.4.

Amino functional groups with two hydrogens and one alkyl group are called **primary amines**. Unlike alcohols, amines are classified as primary, secondary and tertiary according to the number of alkyl groups attached to the nitrogen atom. Secondary and tertiary amines exist, but these compounds are not covered in this course. Some primary amines are shown in Figure 13.2.5.

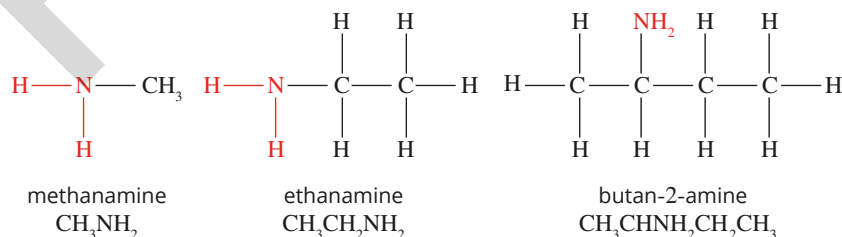


FIGURE 13.2.5 Structural and condensed structural formulae of three primary amines. The amino functional group is shown in red. Primary amines have one carbon atom bonded to the nitrogen atom.

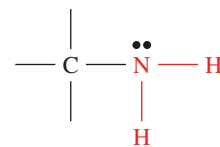


FIGURE 13.2.4 Primary amines contain the amino functional group, -NH₂ (in red). There are two non-bonding electrons on the nitrogen atom.

CHEMFILE

Amines, chocolate and happiness!

An active ingredient in chocolate (Figure 13.2.6) is the primary amine 2-phenylethanamine. 2-Phenylethanamine is also produced in the pleasure centres of the brain and has the effect of generating a general sense of wellbeing or happiness, as well as temporarily raising blood pressure and blood glucose levels.

Eating chocolate provides you with a boost of 2-phenylethanamine, so the reason eating chocolate might make you feel happy is partly due to organic chemistry!



FIGURE 13.2.6 Chocolate contains an amine that makes humans feel happy.

Naming amines

Amines are named in a similar way to alcohols. You can determine the name of an amine as follows.

- Replace the ‘-e’ at the end of the parent alkane’s name with the suffix ‘-amine’.
- If structural isomers are possible, insert a number before ‘-amine’ to indicate the carbon to which the amino functional group is attached.

Table 13.2.3 shows two examples of naming amines.

TABLE 13.2.3 Examples of naming amines

Name	Condensed formula	Structural formula
Ethanamine	$\text{CH}_3\text{CH}_2\text{NH}_2$	<pre> H H H — C — C — N — H H H H</pre>
Butan-2-amine	$\text{CH}_3\text{CHNH}_2\text{CH}_2\text{CH}_3$	<pre> H N — H H H H H H — C — C — C — C — H H H H H</pre>

CARBOXYLIC ACIDS

Formulae and structure of carboxylic acids

Carboxylic acids are a homologous series that contain the carboxyl functional group (Figure 13.2.7). In this functional group, a carbon atom has a double bond to one oxygen atom and a single bond to a second oxygen atom. This second oxygen atom is also bonded to a hydrogen atom. This $-\text{COOH}$ group can be regarded as replacing one hydrogen in the structure of an alkane. The bonds around the carbon atom have a trigonal planar arrangement with the $\text{O}-\text{C}-\text{O}$ angle being about 120° , as shown in Figure 13.2.8.

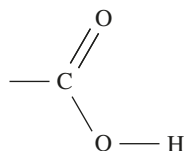


FIGURE 13.2.7 Structure of the carboxyl functional group

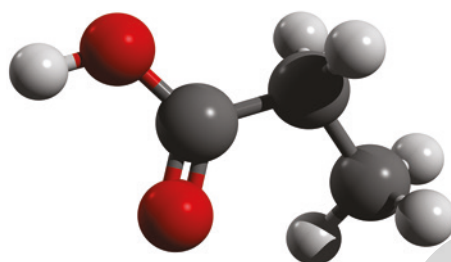


FIGURE 13.2.8 A carboxylic acid has a tetrahedral arrangement of atoms in the hydrocarbon part of the molecule, but there is a trigonal planar arrangement of atoms in the carboxyl functional group.

The **carboxyl functional group** is represented in a condensed formula as $-\text{COOH}$ and is always located at one end of a hydrocarbon chain. Figure 13.2.9 shows the structural and condensed formulae of three carboxylic acids.

Naming carboxylic acids

The prefixes that are used to indicate the number of carbon atoms in alkanes are also used with carboxylic acids. You can determine the name of a carboxylic acid as follows.

- Use the suffix ‘-oic acid’.
- Count the carbons in the functional group in the chain used to name the carboxylic acid. For example, $\text{C}_2\text{H}_5\text{COOH}$ has three carbons and is called propanoic acid.
- Always number the carboxyl carbon as number 1.

The general formula of a carboxylic acid is often represented as RCOOH , where R is an alkyl group such as $-\text{CH}_3$ and $-\text{C}_2\text{H}_5$. The first three members of the carboxylic acid homologous series are listed in Table 13.2.4. Successive members of the series differ by a $-\text{CH}_2-$ unit.

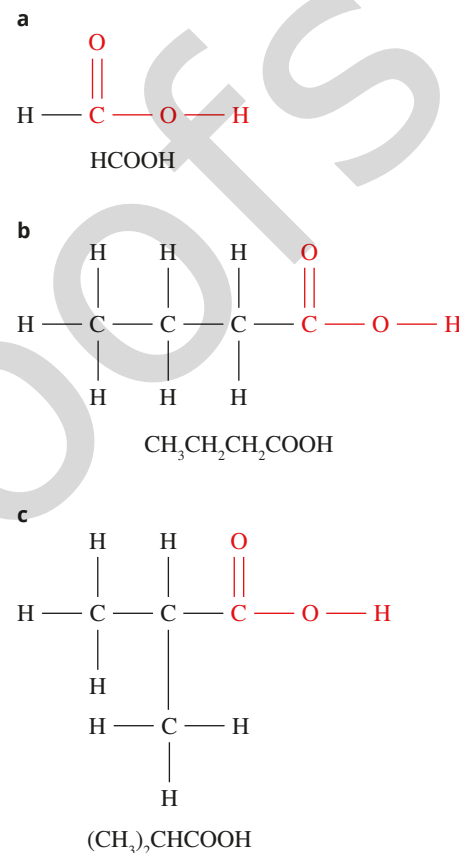


FIGURE 13.2.9 Structural and condensed structural formulae of three carboxylic acids. The carboxyl functional group is shown in red. Note that molecules (b) and (c) are isomers with the molecular formula $\text{C}_4\text{H}_8\text{O}_2$.

TABLE 13.2.4 The first three members of the homologous series of carboxylic acids

Name	Molecular formula	Electron dot formula (Lewis structure)	Structural formula	Condensed structural formula
Methanoic acid	HCOOH			HCOOH
Ethanoic acid	CH_3COOH			CH_3COOH
Propanoic acid	$\text{C}_2\text{H}_5\text{COOH}$			$\text{CH}_3\text{CH}_2\text{COOH}$

Structural isomers of carboxylic acids

The carboxyl group can only occur on the end of a molecule because the carbon atom in the carboxyl group has a double bond to one oxygen and a single bond to another oxygen. Carboxylic acids can form isomers with different branches, but the carbon atom in the carboxyl group is always carbon number 1.

Worked example 13.2.3

IUPAC NAMING SYSTEM FOR CARBOXYLIC ACIDS

Write the systematic name for the following molecule.	
Thinking	Working
Identify the functional group that is present.	There is a carboxyl group present.
Identify the longest carbon chain that includes the carboxyl carbon. This atom will be C1. The stem name of the molecule is based on this longest chain.	There are four carbons in the longest chain, so the stem name is based on butane.
Number the carbon atoms, starting from the end incorporating the functional group.	
Identify the position(s) and the type(s) of branches.	There is a methyl group on C2.
Combine all components. Place the number for the position of the branch in front of the prefix and use the ending -oic acid.	The name of the molecule is 2-methylbutanoic acid.

Worked example: Try yourself 13.2.3

IUPAC NAMING SYSTEM FOR CARBOXYLIC ACIDS

Write the systematic name for the following molecule.

PRIMARY AMIDES

Primary **amides** contain a carbonyl functional group attached to an amino functional group. They are similar to carboxyl groups, except that the $-OH$ is replaced with $-NH_2$ (Figure 13.2.10).

The nitrogen atom in primary amides is bonded to two hydrogen atoms. Secondary and tertiary amides exist, but these compounds are not covered in this course. The **amide functional group** is represented in a condensed formula as

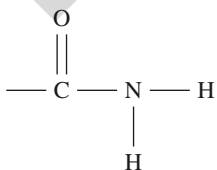


FIGURE 13.2.10 Structure of the amide functional group in a primary amide.

–CONH₂ and is always located at one end of a hydrocarbon chain. The structural and condensed structural formulae of three primary amides are shown in Figure 13.2.11.

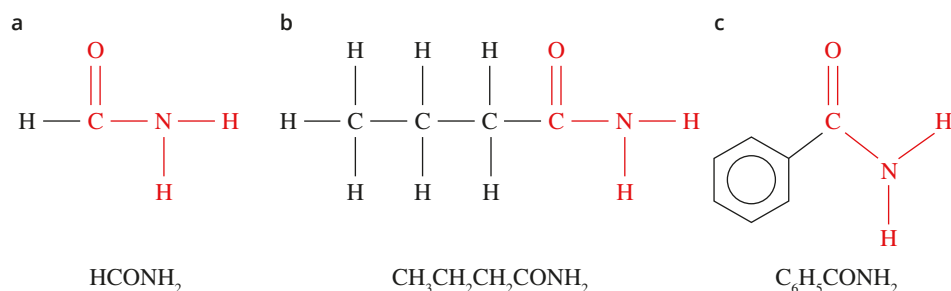


FIGURE 13.2.11 Structural and condensed structural formulae of three amides, with the amide functional group shown in red.

Naming amides

You can determine the name of an amide as follows.

- Identify the length of the parent chain.
- Given the amide group in primary amides is found at one end of the chain, number this carbon as carbon 1.
- Use the prefix for the parent name and add the suffix ‘amide’ to represent this functional group.

For example, in Figure 13.2.11a, the carbon chain is made up of only one carbon and therefore given the prefix meth-. It has only single bonds so the name of this molecule is methanamide. Figure 13.2.11b is called butanamide because it is made up of four carbons and the amide functional group.

CHEMFILE

Urea and organic chemistry

The amide urea ((NH₂)₂CO) is the end product of the breakdown of proteins by mammals and is excreted in urine. This naturally produced urea can be used as a source of nitrogen to promote plant growth (see Figure 13.2.12).

Friedrich Wöhler, a German chemist, synthesised urea in his laboratory in 1828 by treating silver cyanate with ammonium chloride. In a letter to a colleague, Wöhler excitedly wrote: ‘I must tell you that I can make urea without the use of kidneys, either man or dog’.

Wöhler’s synthesis of urea was remarkable because it was the first time someone had made an organic molecule. This discovery established the field of synthetic organic chemistry, which is responsible for millions of products in our society.



FIGURE 13.2.12 Urea is used commercially in fertiliser.

ESTERS

Esters are produced by the reaction of a carboxylic acid with an alcohol. The **ester functional group** (Figure 13.2.13) contains a carbonyl group attached to an oxygen linked to another carbon. It is similar to a carboxyl group, but the hydrogen of the –OH is replaced by an alkyl group.

Figure 13.2.14 shows the structural and condensed structural formulae of three esters. In condensed structural formulae, the ester functional group is usually written as –COO– or –CO₂–

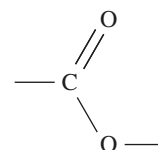


FIGURE 13.2.13 Structure of the ester functional group

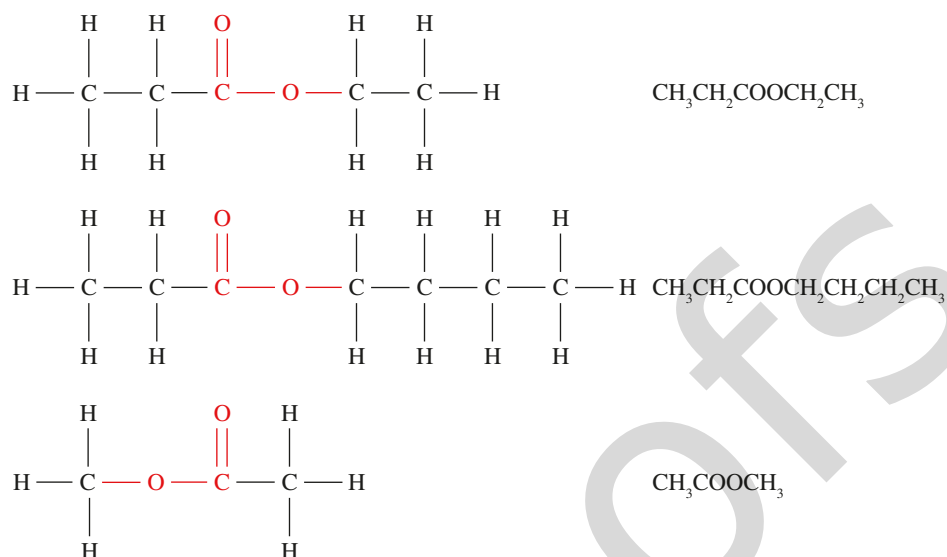


FIGURE 13.2.14 Structural and condensed structural formulae of three esters. Each contains the ester functional group shown in red.

The general formula of an ester may be represented as $\text{R}-\text{COO}-\text{R}'$ where R and R' are alkyl groups, which may or may not be identical.

Esters are formed when carboxylic acids are heated with alcohols in the presence of sulfuric acid. Sulfuric acid acts as a catalyst because it increases the rate of reaction, but is not consumed by the reaction.

In Figure 13.2.15, you can see that an ester functional group is formed from the **esterification reaction** between the carboxyl functional group of the carboxylic acid and the hydroxyl functional group of the alcohol. Because a small molecule (in this case water) is formed in this reaction, the reaction is also a **condensation reaction**.

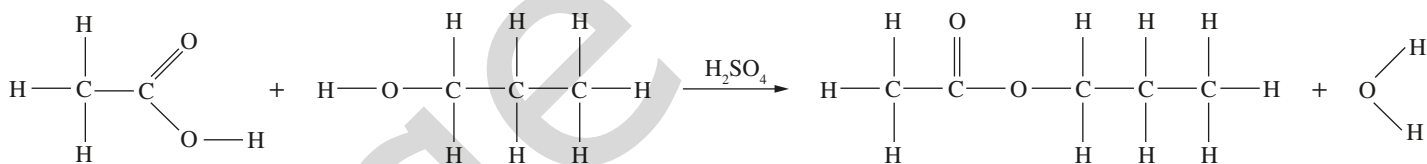


FIGURE 13.2.15 Reaction of a carboxylic acid and an alcohol to form an ester

Naming esters

The name of the ester is made up of the two compounds that react to form the ester—an alcohol and a carboxylic acid, as shown in Figure 13.2.16.

You can determine the name of an ester as follows.

- Locate the functional group and the carbonyl carbon.
- Starting from this carbon, determine the number of carbon atoms in the chain attached to it. Name it according to the stem name, adding the suffix '-oate'. This carbonyl-containing portion of the ester is derived from the carboxylic acid.
- Then add the alkyl group bonded to the singly bonded oxygen atom in front of the name. This portion of the ester is derived from the alcohol.

Use Worked Example 13.2.4 to develop your skills in naming esters.

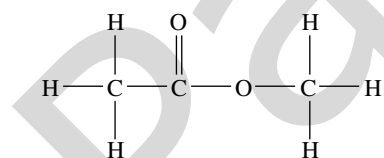
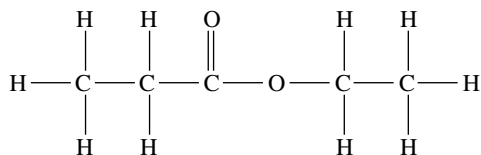


FIGURE 13.2.16 Methyl ethanoate (acetate) is an ester formed by the reaction of methanol with ethanoic acid.

Worked example 13.2.4

IUPAC NAMING SYSTEM FOR ESTERS

Write the systematic name for the following molecule.



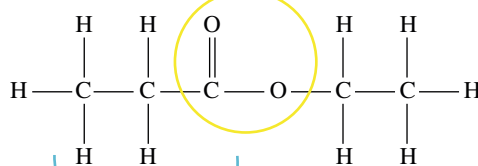
Thinking

Locate the ester functional group.

Starting from the carbonyl carbon, determine the number of carbon atoms in the chain attached to it and name according to the stem name, adding the suffix '-oate'.

Working

ester functional group

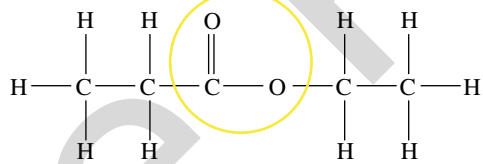


3 C atoms including the carbonyl carbon

There are three carbons in the chain, including the carbonyl carbon, so the last part of the ester's name is propanoate.

Count how many carbons are bonded to the singly bonded oxygen atom. The alkyl group bonded to the singly bonded oxygen atom is then added in front of the name.

ester functional group



2 C atoms bonded to the singly bonded oxygen atom

There are two carbon atoms bonded to the singly bonded oxygen atom, so the alkyl group is ethyl.

Combine the two components, placing the alkyl part of the name first.

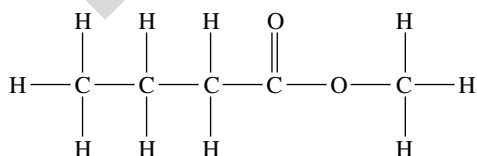
The name of the molecule is ethyl propanoate.

i The name of the ester can easily be determined if you know the names of the carboxylic acid and alcohol that it is made from. The alkyl group name is derived from the name of the alcohol; for example, methanol becomes methyl. The -oic acid portion of the carboxylic acid name is replaced with -oate; for example, ethanoic (acetic) acid becomes ethanoate (acetate). The name of the example ester would be methyl ethanoate.

Worked example: Try yourself 13.2.4

IUPAC NAMING SYSTEM FOR ESTERS

Write the systematic name for the following molecule.



Structural isomers of esters

The position of the ester group can vary within a molecule and create structural isomers. Figure 13.2.17 shows three esters that are structural isomers with the molecular formula, $C_5H_{10}O_2$. The position of the ester functional group is shown by the naming of the ester, rather than by using numbers.

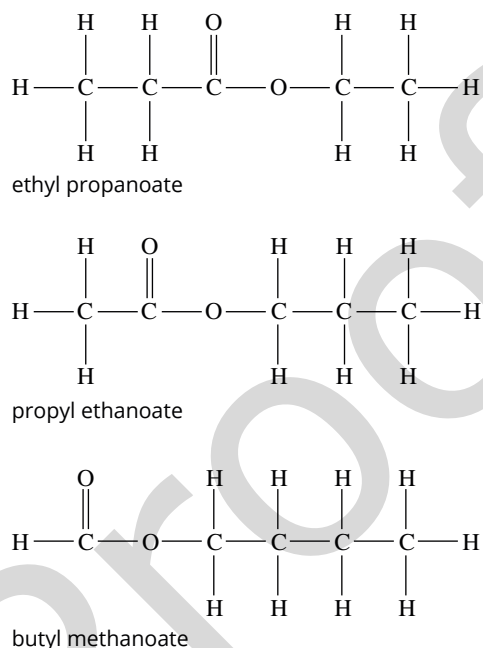


FIGURE 13.2.17 Three esters that are structural isomers with the molecular formula $C_5H_{10}O_2$

ALDEHYDES AND KETONES

Molecules of aldehydes, ketones, carboxylic acids, amides and esters all contain a **carbonyl functional group** as shown in Figure 13.2.18. A carbonyl functional group consists of a carbon atom connected to an oxygen atom by a double bond. All atoms bonded to the carbon atom are in a plane and the angles between bonds are 120° .

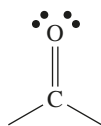


FIGURE 13.2.18 The carbonyl functional group. The non-bonding pairs of electrons shown on the oxygen atom are often not included in structural formulae.

Aldehydes

In **aldehydes**, the carbonyl group is always at the end of the hydrocarbon chain. As shown in Figure 13.2.19, the carbon atom of the carbonyl group is bonded to a hydrogen atom. The carbonyl functional group in an aldehyde is always written as $-CHO$ at the end of the condensed structural formula of aldehydes.

The simplest aldehyde, methanal ($HCHO$), is also commonly known as formaldehyde and is used to preserve biological specimens, including embalming human remains.

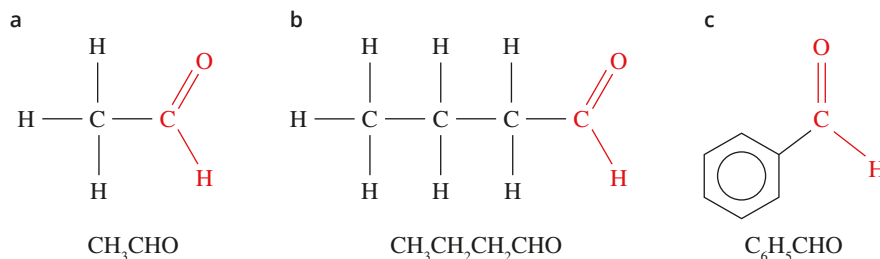


FIGURE 13.2.19 Structural and condensed formulae of three aldehydes. Each contains a carbonyl functional group with a hydrogen atom attached, shown in red.

Naming aldehydes

You can determine the name of an aldehyde as follows.

- Locate the functional group and the carbonyl carbon.
- Starting from this carbon, determine the number of carbon atoms in the chain attached to it. Name it according to the stem name, adding the suffix ‘-al’.

For example, the structure in Figure 13.2.19a has two carbons in the chain, so is given the prefix ‘ethan-’. Being an aldehyde, it is given the suffix ‘-al’. Therefore, the name of this aldehyde is ethanal. Figure 13.2.19b is composed of a chain made up of four carbon atoms with the carbonyl hydrocarbon. Therefore, it is called butanal.

Ketones

In **ketones**, the carbonyl carbon is attached to other carbon atoms. This means that the carbonyl group is never at the end of the molecule, as you can see in the examples in Figure 13.2.20. In condensed structural formulae, the carbonyl functional group in a ketone is simply written as -CO- .

The simplest ketone, propanone (CH_3COCH_3), is commonly called acetone and is a useful polar organic solvent, frequently found in nail polish remover and paint thinner.

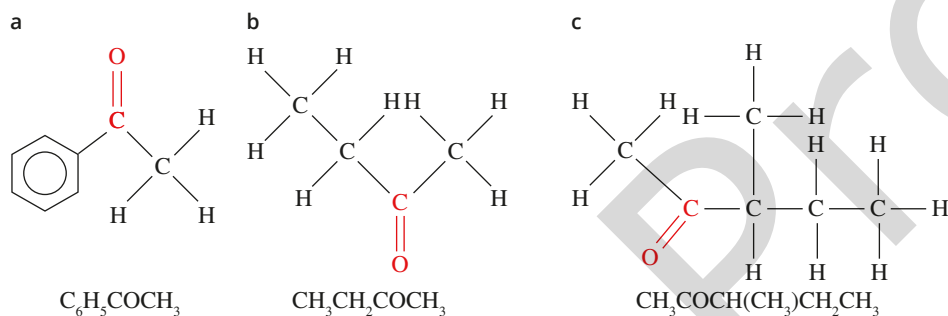


FIGURE 13.2.20 Structural and condensed formulae of three ketones. Each contains a carbonyl functional group (shown in red) attached to two hydrocarbon groups.

Naming ketones

You can determine the name of a ketone as follows.

- Identify the end of the hydrocarbon chain closest to the functional group and number the carbons from this end of the molecule.
- If there is a branched alkane, write the number and name of the alkyl group.
- Use the prefix for the number of carbon atoms present in the chain and suffix ‘-one’, indicating the position of the double bonded oxygen by inserting the number between the prefix and suffix in the final part of the name.

For example, in Figure 13.2.20b, the chain is four carbons long. The position of the carbonyl group is attached to the second carbon so this is butanone. Figure 13.2.20c has a methyl group attached to the third carbon in the chain. This ketone is named 3-methyl-2-pentanone.

Figure 13.2.20a has a benzene group as well as a methyl group. The chain is essentially the same as propanone with a benzene ring making up the position of the third carbon in the chain. It is given the name 1-phenylethan-1-one. This name has a prefix of phenyl to indicate the benzene ring and overall ‘-one’ suffix to indicate the presence of the carbonyl group.

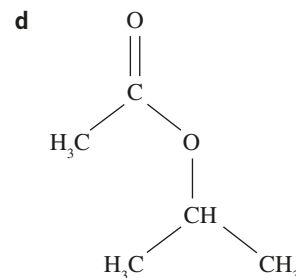
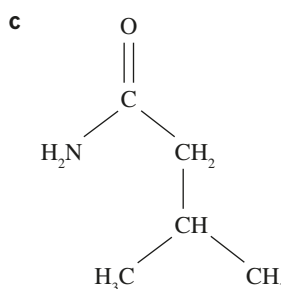
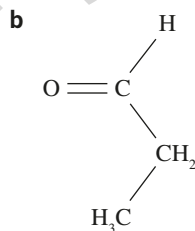
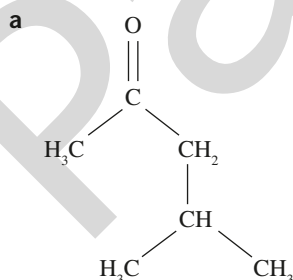
13.2 Review

SUMMARY

- Alcohols are a homologous series that contain a hydroxyl ($-\text{OH}$) group.
 - Alcohols are named by replacing the 'e' at the end of the parent alkane with the suffix '-ol'.
 - Alcohols are differentiated from each other as primary, secondary or tertiary alcohols depending on the number of alkyl groups to which they are bonded.
- Primary amines are a homologous series which contain an amino ($-\text{NH}_2$) functional group.
 - Primary amines are named by replacing the 'e' at the end of the parent alkane with the suffix '-amine'.
- When isomers exist, a number is used to specify the position of the functional group.
- The carbonyl group ($-\text{CO}-$) is a component of a number of functional groups.
- Aldehydes and ketones are homologous series that contain a carbonyl group on its own.
 - Aldehydes are named by replacing the 'e' at the end of the parent alkane with the suffix '-al'.
 - Ketones are named using with the suffix '-one', with a number used to identify the position of the carbonyl group.
- The carbonyl group is at the end of a hydrocarbon chain in aldehydes and within a hydrocarbon chain in ketones.
- Carboxylic acids are a homologous series of molecules that contain the carboxyl group ($-\text{COOH}$) at the end of a hydrocarbon chain.
 - Carboxylic acids are named using the suffix '-oic acid'.
- Primary amides are a homologous series of molecules that contain the amide group ($-\text{CONH}_2$) at the end of the hydrocarbon chain.
- Esters are a homologous series of molecules that contain an ester group ($-\text{COO}-$) within the hydrocarbon chain.
- Esters have a two-word name.
 - The first part of the name comes from the part derived from an alcohol and the '-ol' suffix is changed to '-yl'.
 - The second part of the name is derived from the part that comes from a carboxylic acid and the suffix '-oic acid' is changed to '-oate'.

KEY QUESTIONS

- Draw the structure and then write the name of a tertiary alcohol with the molecular formula $\text{C}_5\text{H}_{12}\text{O}$.
- Give the systematic names of:
 - $\text{CH}_3(\text{CH}_2)_3\text{CH}_2\text{OH}$
 - $\text{CH}_3(\text{CH}_2)_3\text{CHNH}_2(\text{CH}_2)_2\text{CH}_3$
- What homologous series do each of the following molecules belong to?



- Write the systematic name for the following molecules.
 - HCOOCH_3
 - HCOOH
 - $\text{CH}_3\text{CH}_2\text{CH}_2\text{COOCH}_2\text{CH}_2\text{CH}_3$
 - $\text{CH}_3\text{COOCH}_3$
 - $\text{CH}_3(\text{CH}_2)_4\text{COOCH}_2\text{CH}_3$
- Draw and name an isomer of HCOOCH_3 .

13.3 Properties of organic compounds

The functional groups that are present in organic compounds are responsible for many of their chemical and physical properties. For example, the properties of methanoic acid (formic acid, HCOOH) (Figure 13.3.1) are largely determined by the presence of the polar, acidic carboxyl functional group in its molecules.



FIGURE 13.3.1 Green tree ants weave leaf nests in the Gardner Plateau on the Kimberley Coast in Western Australia. Weaver ants can inflict painful bites and often spray methanoic acid directly at the bite wound, resulting in intense discomfort.

In this section you will consider the effect of functional groups on physical properties such as boiling point, solubility and viscosity. Differences in chemical properties will also be linked to the ability of functional groups to form different intermolecular interactions.

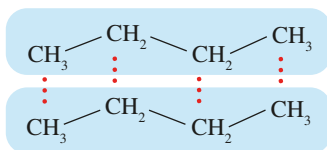
PHYSICAL PROPERTIES OF ALKANES AND ALKENES

Boiling points of alkanes

Table 13.3.1 lists the boiling points of the first six alkanes from methane to hexane. The boiling points increase as the size of the alkane molecule increases.

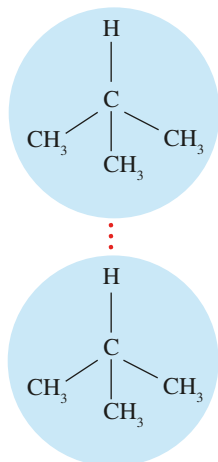
TABLE 13.3.1 Boiling points of the first six alkanes

Alkane	Molecular formula	Boiling point (°C)
Methane	CH ₄	-162
Ethane	C ₂ H ₆	-89
Propane	C ₃ H ₈	-45
Butane	C ₄ H ₁₀	-0.5
Pentane	C ₅ H ₁₂	36
Hexane	C ₆ H ₁₄	69



butane

- less compact molecule
- molecules are closer
- boiling point -0.5°C



methylpropane

- more compact molecule
- molecules are further apart
- boiling point -11.7°C

FIGURE 13.3.3 Molecular shape affects boiling point. Dispersion forces between butane molecules are stronger than those between methylpropane molecules because butane molecules are less compact and can come closer together.

Because alkane molecules are non-polar, the only intermolecular forces of attraction between them are weak **dispersion forces**. As the length of the carbon chain increases, the overall forces of attraction between molecules also increase (Figure 13.3.2). The dispersion forces between molecules increase because of the increased strength of temporary dipoles within the molecules. Because the boiling point of a molecular substance is determined by the strength of the intermolecular forces, boiling points increase as alkane chain length increases.

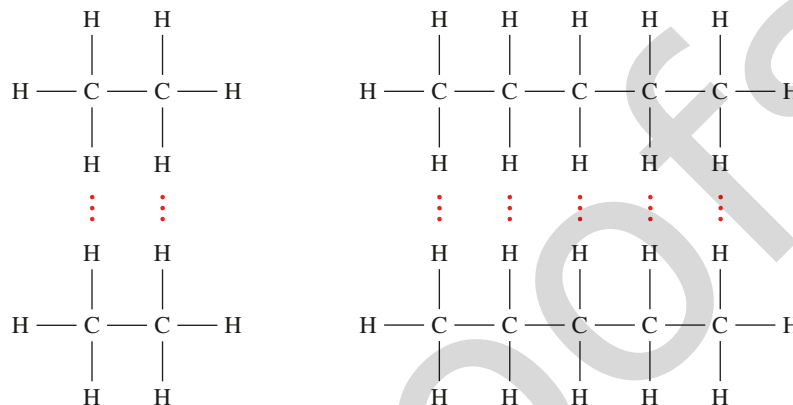


FIGURE 13.3.2 Dispersion forces are the strongest forces between alkane molecules. As molecules become longer, the dispersion forces become stronger.

Molecular shape also influences the strength of dispersion forces and, therefore, boiling points. Straight-chain alkanes are able to fit together more closely and tend to have higher boiling points than their corresponding branched-chain isomers, which are unable to come as close together in the bulk substance.

Figure 13.3.3 shows how the shapes of butane and its branched isomer methylpropane influence the strength of the dispersion forces between the molecules. Butane ($\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$) boils at -0.5°C , whereas methylpropane ($(\text{CH}_3)_3\text{CH}$) boils at -11.7°C . Although both molecules have the same molecular formula of C_4H_{10} , molecules of $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ have a greater surface area and can fit more closely together, allowing more contact between the molecules and form stronger intermolecular bonds.

i The strength of dispersion forces between molecules depends on the size and shape of the molecules.

Boiling points of alkenes

Alkenes are non-polar and the forces of attraction between them are only weak dispersion forces. As you can see in Table 13.3.2, members of this homologous series have relatively low boiling points, similar to those observed for the alkanes with the same number of carbon atoms.

As for the alkanes, the boiling points of alkenes increase with molecular size as the strength of dispersion forces between molecules increases.

TABLE 13.3.2 Boiling points of molecules containing four carbons with different functional groups

Compound	Boiling point ($^{\circ}\text{C}$)
Butane (C_4H_{10})	-0.5
But-1-ene (C_4H_8)	-6.3
But-1-yne (C_4H_6)	-8.1

CHEMFILE

Have you got the patience for slow science?

The longest running laboratory experiment in the world was set up in 1927 at the University of Queensland in Brisbane. The long-running 'pitch drop' experiment is designed to show that pitch, a mixture of highly viscous hydrocarbons, is actually a liquid. Pitch, otherwise known as bitumen (Figure 13.3.4), appears solid on first inspection and shatters if you strike it with a hammer.

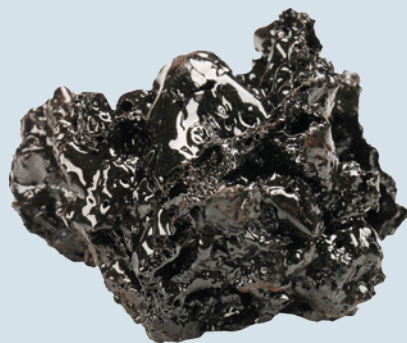


FIGURE 13.3.4 A sample of pitch at room temperature appears solid and shatters when hit with a hammer.

Professor Thomas Purnell set up the pitch experiment as shown in Figure 13.3.5 by placing a sample of pitch into a funnel encased in a sealed container. He wanted to demonstrate to students that pitch was indeed a liquid—just a very, very viscous one. Over time, the pitch has settled and slowly flowed through the funnel, producing on average a drop once every decade. The ninth drop was recorded in April of 2014.

Today, bitumen is used extensively, forming the main component of road surfaces. Under normal conditions, the road surface appears solid. However, heating reduces the viscosity and road workers are able to work the pliable bitumen.



FIGURE 13.3.5 Professor Thomas Purnell set up the famous University of Queensland pitch drop experiment in 1927. Professor John Mainstone, shown here, oversaw the experiment for many years.

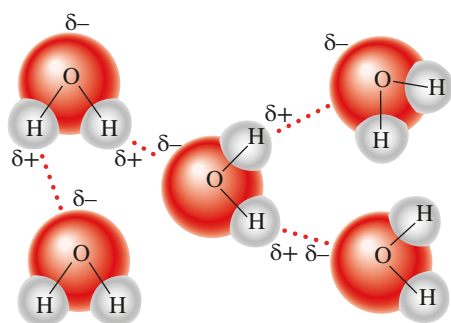


FIGURE 13.3.6 Water molecules are held to each other by hydrogen bonding.

Solubility in water

The non-polar nature of alkanes and alkenes makes them insoluble in water. You will recall from Year 11 Chemistry that water molecules are polar and held together by strong **hydrogen bonds** (Figure 13.3.6). The weak dispersion forces between water molecules and hydrocarbon molecules are not strong enough to overcome the strong attraction between water molecules so the two substances remain separate and do not mix.

For example, when hexane is added to water, it simply forms a layer on top of the water because hexane is less dense than water and the two liquids cannot dissolve in each other. Liquids that do not mix are said to be **immiscible**.

Crude oil is a mixture of many different compounds. Most of these compounds are hydrocarbon compounds of varying lengths. While there are some alkenes in crude oil, many of the hydrocarbons are alkanes. Because alkanes are generally less dense than water, when crude oil spills occur at sea the crude oil floats on the surface, forming a thick insoluble layer. As the oil layer is moved by the waves of the sea, the oil can spread over many hundreds of square kilometres. The presence of the thick oil layer can have disastrous consequences for marine and bird life. Oil that reaches the shore, like the oil spill shown in Figure 13.3.7, has drastic effects on beaches and wildlife.



FIGURE 13.3.7 Oil spills at sea can contaminate shorelines and are very difficult to clean due to the lack of solubility of the oil in water. Other non-polar solvents or physical methods are required to disperse or remove the oil.



FIGURE 13.3.8 White spirit contains a mixture of alkanes. It is a useful solvent for other non-polar liquids.

Solubility in organic solvents

Alkanes mix with other non-polar liquids such as alkenes and symmetrical haloalkanes. This is because the forces of attraction between molecules of these liquids are also weak dispersion forces and of similar strength to the alkane–alkane forces of attraction. Therefore, these liquids are **miscible**; that is, they are soluble in each other.

Many commercial cleaning agents contain non-polar liquids that are useful for removing oil stains. White spirit is a mixture of alkanes and other hydrocarbons obtained by the refining of crude oil. White spirit is a useful cleaning agent because it can dissolve other non-polar liquids, such as oils and greases. It is used as a solvent in aerosols and in the home as a degreasing solvent. White spirit is also used for cleaning paintbrushes and as a general cleaning agent (Figure 13.3.8).

PHYSICAL PROPERTIES OF ALCOHOLS, CARBOXYLIC ACIDS, AMINES AND AMIDES

Compounds from the four homologous series alcohols, carboxylic acids, amines and amides will be considered together because their molecules contain functional groups that can form hydrogen bonds. The ability of molecules to form hydrogen bonds has a significant effect on their properties.

Boiling points

Hydrogen bonds are the strongest of the intermolecular forces and, as a result, molecules that can form hydrogen bonds generally exhibit higher boiling points. You can see in Table 13.3.3 that alcohols, carboxylic acids, amines and amides have higher boiling points than alkanes of similar molecular mass.

TABLE 13.3.3 Comparison of boiling points of compounds with different functional groups based on molecular mass

Homologous series	Compound	Formula	Molar mass (g mol^{-1})	Boiling point ($^{\circ}\text{C}$)
Alkane	Butane	C_4H_{10}	58	-1
Alcohol	Propan-1-ol	$\text{C}_3\text{H}_7\text{OH}$	60	97.2
Carboxylic acid	Ethanoic acid	CH_3COOH	60	118
Amine	Propan-1-amine	$\text{C}_3\text{H}_7\text{NH}_2$	59	49
Amide	Ethanamide	CH_3CONH_2	59	210

Boiling points of alcohols

The higher boiling points of the alcohols are due to the presence of hydrogen bonds between neighbouring alcohol molecules. In contrast, the only type of bonding present between non-polar alkane molecules is much weaker dispersion forces.

You will recall from Year 11 Chemistry that oxygen is a more **electronegative** atom than hydrogen, so the oxygen-hydrogen bond in the hydroxyl functional group is a polar bond. Figure 13.3.9 shows how hydrogen bonding occurs between the partially charged hydrogen atom in the $-\text{OH}$ group on one alcohol molecule and a non-bonding electron pair on the oxygen atom of a neighbouring alcohol molecule. The presence of the hydrogen bonds results in the higher boiling points observed.

Boiling points of amines and amides

The presence of highly polar nitrogen-hydrogen bonds in amine and amide molecules means that these molecules can also form hydrogen bonds. The formation of hydrogen bonds between amines and amides is illustrated in Figure 13.3.10.

i The addition of polar functional groups to a hydrocarbon increases the boiling point for molecules of a similar size compared to the non-polar alkanes.

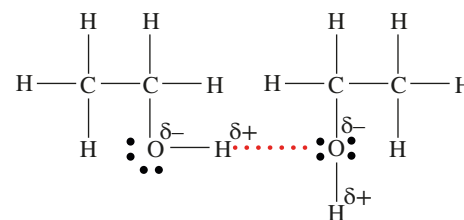


FIGURE 13.3.9 The red dotted line shows the hydrogen bonds that form between molecules such as ethanol that contain the polar hydroxyl functional group.

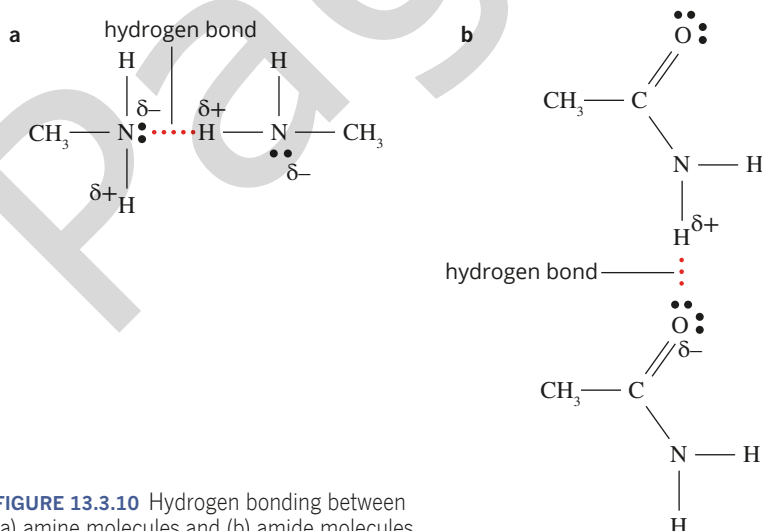


FIGURE 13.3.10 Hydrogen bonding between (a) amine molecules and (b) amide molecules.

In amines, the hydrogen bonds form between the non-bonding pair of electrons on the electronegative nitrogen atom and the partially positive hydrogen atom on another amine molecule. In amides, hydrogen bonds form between the non-bonding electron pairs on the oxygen atoms of one molecule and the partially positive hydrogen atom on a neighbouring molecule. The strength of the hydrogen bonding between molecules explains the relatively high boiling points of amines and amides when compared to hydrocarbon molecules of similar size.

Boiling points of carboxylic acids

Hydrogen bonding also has a marked effect on the boiling points of carboxylic acids. Figure 13.3.11 shows how two molecules of a carboxylic acid in the liquid state can form dimers in which two hydrogen bonds form between the molecules.

The dimer produced is a stable species with a molar mass that is double that of a single carboxylic acid molecule. The increase in size that results from the formation of the dimer increases the strength of the dispersion forces between one dimer and its neighbours. The higher dispersion forces combined with the hydrogen bonds between molecules results in the higher boiling point observed for carboxylic acids when compared to most other organic molecules of similar size.

Figure 13.3.12 highlights the higher boiling points of the carboxylic acid homologous series compared to alcohols.

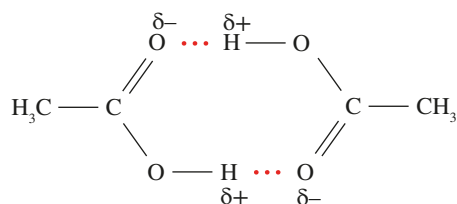


FIGURE 13.3.11 Hydrogen bonding between two ethanoic acid molecules results in the formation of a dimer.

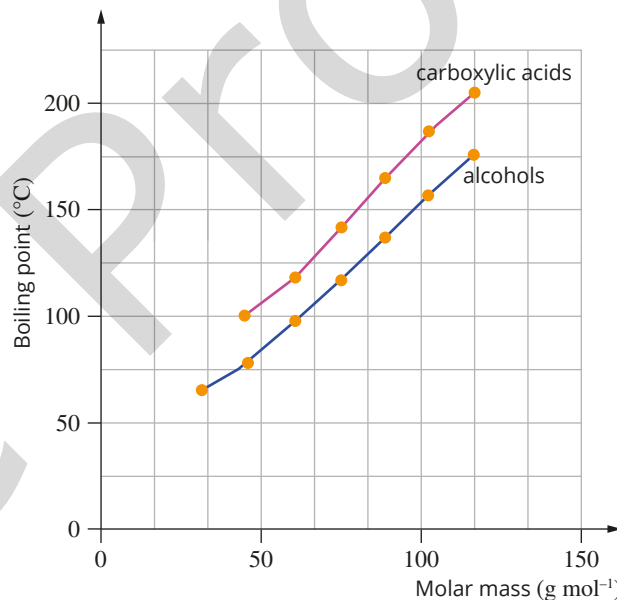


FIGURE 13.3.12 Boiling points of the carboxylic acid homologous series increases with increasing molar mass. The boiling points are higher than the boiling points of alcohols because of the formation of dimers stabilised by hydrogen bonds between molecules.

Effect of chain length on boiling point

The boiling points of alcohols, amines, amides and carboxylic acids increase as molar mass increases. For example, in alcohols the intermolecular hydrogen bonding between the $-OH$ groups results in the higher boiling points. As the length of the hydrocarbon chain or 'tail' increases from one member of the homologous series to the next, the molar mass of the alcohols increases. With the increase in molecular size, the dispersion forces between molecules also get stronger. So the boiling points of alcohols increase as molar mass increases (Figure 13.3.13).

The three-dimensional structure of molecules can also affect the boiling point of a compound. In the case of alcohols, in addition to the impact of branching on the strength of dispersion forces, the position of the hydroxyl group within the molecule affects the hydrogen bonding. Figure 13.3.13 shows molecular models for three isomers of butanol: butan-1-ol, butan-2-ol and 2-methylpropan-2-ol. These isomers are examples of primary, secondary and tertiary alcohols, respectively.

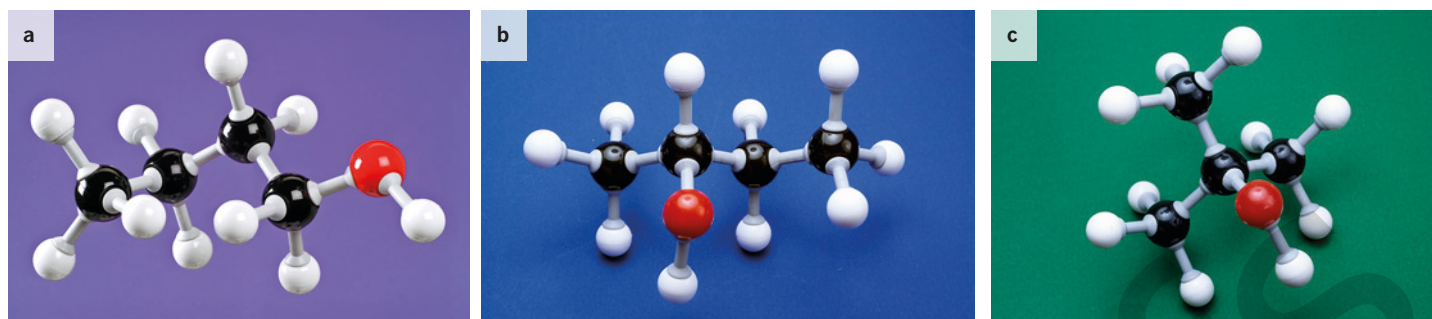


FIGURE 13.3.13 Molecular models of the three isomers of butanol: (a) butan-1-ol, (b) butan-2-ol and (c) 2-methylpropan-2-ol

You can see from the models that the hydroxyl group becomes increasingly 'crowded' from the primary alcohol through to the secondary and tertiary alcohol isomers. The presence of the alkyl groups restricts a molecule's ability to form hydrogen bonds with other molecules. For this reason, the boiling points of these alcohols decrease in the sequence from primary to secondary to tertiary alcohol, as seen in Table 13.3.4.

TABLE 13.3.4 The boiling point of primary, secondary and tertiary alcohols with the formula C_4H_9OH

Alcohol	Type of alcohol	Boiling point ($^{\circ}C$)
Butan-1-ol	Primary	118
Butan-2-ol	Secondary	100
2-Methylpropan-2-ol	Tertiary	82

Solubility

Solubility in water

Small alcohols and amines dissolve well in water because hydrogen bonds can form between the polar functional groups of the molecules and adjacent water molecules. For alcohols, the hydrogen bonds form between the partially positive hydrogen atom of the hydroxyl group and the lone-pair electrons of an adjacent water molecule (Figure 13.3.14a). There is also attraction between the partially positive hydrogen within the water molecules and the lone-pair electrons on the alcohol. This is how ethanol dissolves in water in alcoholic drinks, such as beer or wine.

When amines interact with water molecules (Figure 13.3.14b), hydrogen bonds can form between the lone-pair electrons of the nitrogen and the partial positive hydrogen of an adjacent water molecule or between the hydrogen of an amine group and an oxygen of an adjacent water molecule.

Amide and carboxylic acid molecules with short carbon chains are also soluble in water. When carboxylic acids dissolve in water, hydrogen bonding occurs between water molecules and both the $C=O$ group and the $-OH$ group, making these compounds more soluble than alcohols in water (Figure 13.3.15).

The high solubility of the carboxylic acid, citric acid, and the substance vitamin C, means they are found in a range of solutions, such as orange and lemon juice (Figure 13.3.16).

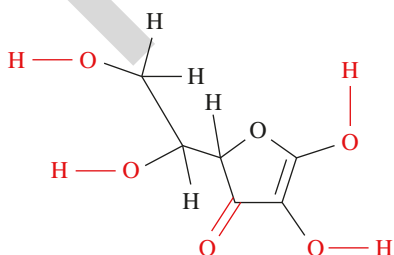


FIGURE 13.3.16 The presence of a large number of polar carbonyl and hydroxyl functional groups in a molecule of vitamin C makes it highly soluble in water. (Carbon atoms in the structure have been omitted for clarity.)

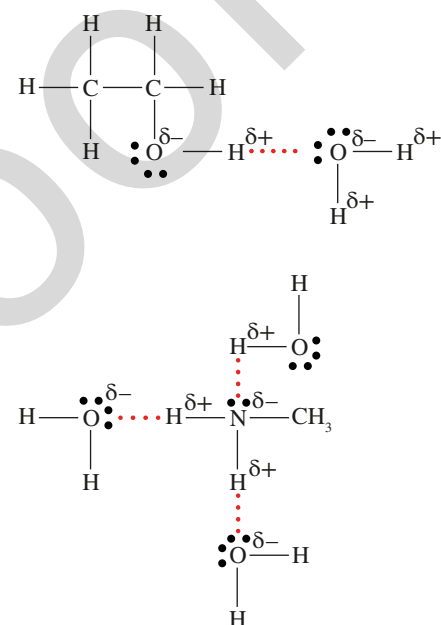


FIGURE 13.3.14 Hydrogen bonding between water molecules and (a) an ethanol molecule and (b) an amine molecule.

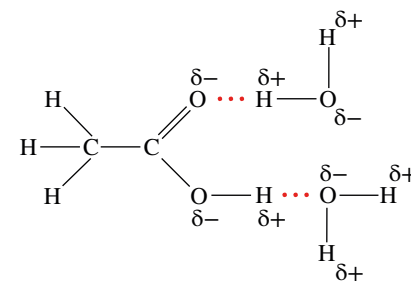


FIGURE 13.3.15 A small carboxylic acid molecule, such as ethanoic acid, is soluble in water due to hydrogen bonding between the carboxyl functional group and water molecules.

Solubility and chain length

The graph in Figure 13.3.17 shows the solubility of three alcohols. The solubility of alcohols, amines, amides and carboxylic acids in water decreases with increasing length of the carbon chain.

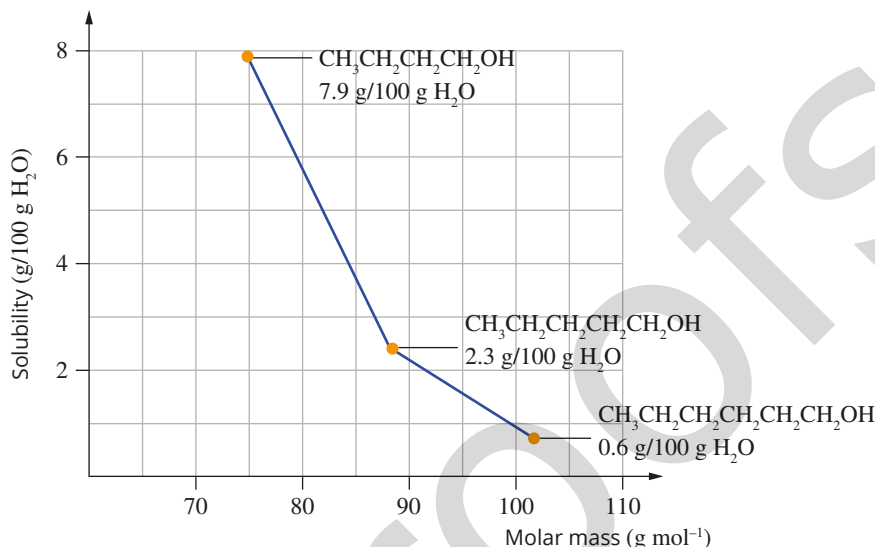


FIGURE 13.3.17 The solubility of alcohols in water decreases with increasing carbon chain length. This trend is also observed for other polar hydrocarbons such as amines, amides and carboxylic acids.

The longer hydrocarbon chains disrupt the hydrogen bonds between water molecules. While the hydroxyl group of an alcohol, for example, can form hydrogen bonds with water molecules, the hydrocarbon ‘tail’ cannot. Only dispersion forces occur between the hydrocarbon chain and water molecules, which are not as strong as hydrogen bonds, opposing the tendency for the molecule to dissolve. As chain length increases, the non-polar nature of the molecule also increases and the alcohol becomes less soluble.

Solubility in organic solvents

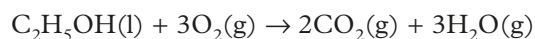
In contrast to their solubility in water, alcohols become more soluble in organic solvents as they get larger. This is because organic solvents—such as hexane, benzene and toluene—are non-polar. Only relatively non-polar alcohols with long hydrocarbon chains dissolve well in non-polar solvents.

Small alcohols such as ethanol, which are very soluble in water, do not dissolve as well in organic solvents. The dispersion forces between their hydrocarbon chains and the solvent are not strong enough to disrupt the hydrogen bonds that hold the alcohol molecules together. Therefore, the alcohol molecules do not separate and disperse throughout the solvent.

The solubilities of amines, amides and carboxylic acids in organic solvents show similar trends to those of alcohols.

Properties and uses of alcohols

Many small alcohols are useful as fuels. Ethanol can be used as a fuel on its own or mixed with petrol. The combustion of ethanol produces carbon dioxide and water:



The boiling points of alcohols increase as the size of the alcohol molecule increases. However, the boiling points of the alcohols are all higher than those of the corresponding alkanes. All the alcohols are liquids at room temperature, in contrast to the alkanes and alkenes, many of which are gases. The trend in boiling points of the first six alcohols is shown in Figure 13.3.18.

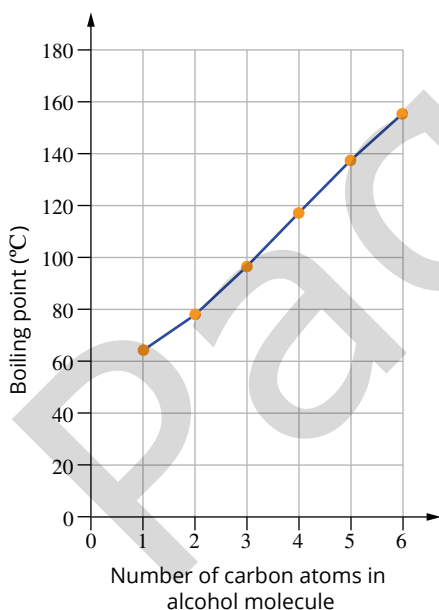


FIGURE 13.3.18 As the number of carbon atoms in an alcohol molecule increases, the boiling point increases.

The higher boiling point of alcohols is due to the presence of the -OH group, which allows hydrogen bonding to occur between molecules and strengthens the intermolecular bonding.

Hydrogen bonding also influences the solubility of the alcohols in water. The presence of the -OH group allows hydrogen bonds to form between water molecules and alcohol molecules (Figure 13.3.19). For smaller alcohols, such as methanol and ethanol, this allows the alcohol to dissolve readily in water. The solubility of the other alcohols decreases as the length of the carbon chain attached to the -OH group increases. A longer carbon chain means that more of the molecule is non-polar and the molecule becomes less polar overall.

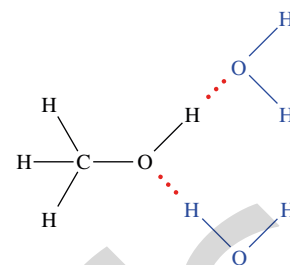
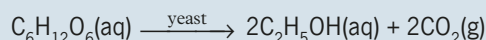


FIGURE 13.3.19 Hydrogen bonds form between the hydroxyl group of a methanol molecule and water.

CHEMFILE

Making champagne

The solubility of ethanol in water is essential in the production of alcoholic drinks. Champagne and wine are made by the fermentation of glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) obtained from grapes. In the presence of yeast, ethanol and carbon dioxide are formed:



When a carefully selected mixture of grapes is fermented in bottles to make champagne, the ethanol and some carbon dioxide dissolves in the aqueous solution. Because the sparkle of the carbon dioxide is required in the final product, the yeast must be removed from the bottles very carefully while keeping the carbon dioxide in solution.

When it is time to remove the yeast from the fermented champagne solution, the bottle is inverted and the yeast is frozen in the neck of the bottle (Figure 13.3.20). The stopper and yeast are then removed quickly and the stopper is replaced.



FIGURE 13.3.20 An inverted bottle of champagne in the Moët & Chandon champagne cellar, Epervay, France. The yeast can be seen near the temporary cap of the bottle.

Properties and uses of carboxylic acids

Carboxylic acids are organic acids. They are commonly found in nature, giving a sour taste to lemon juice and vinegar, or making an ant bite or a nettle prick sting (see Figure 13.3.21 for the structures of these carboxylic acids).

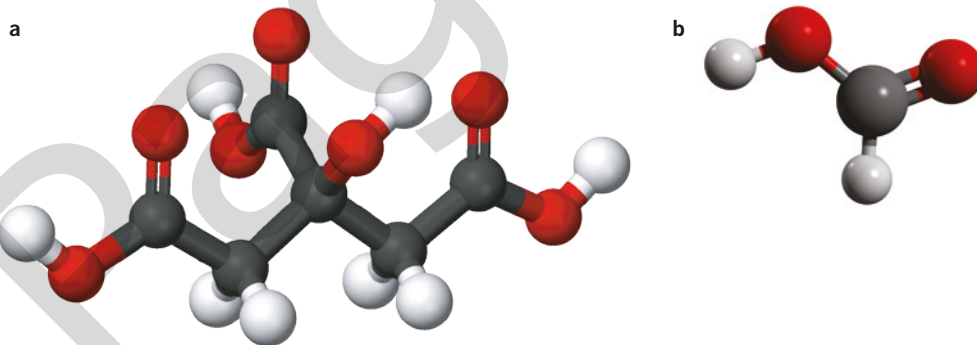


FIGURE 13.3.21 Carboxylic acids are found in nature. (a) Citric acid is in lemons and (b) methanoic acid is present in stinging nettles and ants.

As shown in Figure 13.3.22, the carboxyl functional group is made up of a **carbonyl group** (C=O) and a hydroxyl (-OH) group. Both of these groups are polar, with oxygen being much more electronegative than carbon and hydrogen. The electrons are drawn away from the hydrogen atom, enabling it to react in water to form an $\text{H}^+(\text{aq})$ ion, so the functional group can act as an acid.

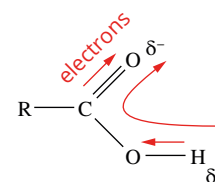


FIGURE 13.3.22 Electrons are drawn away from the hydrogen of the carboxyl functional group, allowing the hydrogen to be donated as a H^+ ion in an acid–base reaction.

CHEMFILE

Butter bombs

When butter goes rancid, the unpleasant odour is due to butanoic acid that has been released from the fats in the butter.

In its pursuit of Japanese whaling ships between 2005 and 2010, the crew of Sea Shepherd ships threw stink bombs made of rancid butter onto the decks of the whaling ships (Figure 13.3.23). While the members of Sea Shepherd maintained that they were throwing essentially harmless food material at the manned whaling ships, the butanoic acid in the rancid butter would not be a pleasant material to get in your eyes.



FIGURE 13.3.23 Sea Shepherd crew members throw butanoic acid in the form of rancid butter onto a Japanese whaling ship.

Carboxylic acids are weak acids and are often found in food. When foods go bad, carboxylic acids can be formed. For example, ethanoic acid is produced when wine is left open to oxygen in the atmosphere. We describe the taste of this wine as ‘vinegary’ because it actually has changed to vinegar. This reaction is used deliberately in the manufacture of the many different varieties of vinegar, such as apple cider vinegar.

PHYSICAL PROPERTIES OF ALDEHYDES, KETONES AND ESTERS

Aldehydes, ketones and esters can be considered together because they are composed of molecules that are held together by dipole–dipole attractions. Their molecules cannot form hydrogen bonds with each other because they do not have a hydrogen atom bonded to an oxygen atom or a nitrogen atom in their molecules.

Boiling points

Aldehydes, ketones and esters all contain a carbon–oxygen double bond. Oxygen is much more electronegative than carbon, so the carbon–oxygen double bond is polar. This means that molecules of aldehydes, ketones and esters contain a permanent dipole, which can form dipole–dipole attractions with nearby molecules. The dipole–dipole interactions that arise between ketone molecules are shown in Figure 13.3.24.

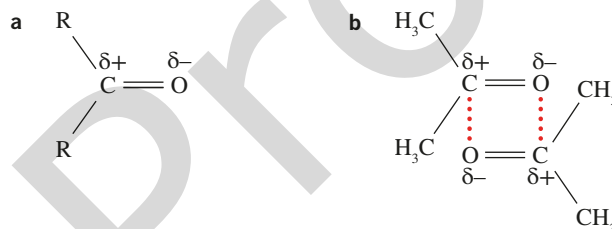


FIGURE 13.3.24 (a) A carbonyl bond is polar. (b) Dipole–dipole attractions between ketone molecules.

The strength of these dipole–dipole bonds between molecules give aldehydes, ketones and esters higher boiling points than similar sized alkanes. However, their boiling points are not as high as similar-sized alcohols because dipole–dipole bonds are not as strong as hydrogen bonds.

Effect of chain length on boiling point

As the hydrocarbon chain of aldehydes, ketones and esters increases in length, their boiling points increase because the strength of the dispersion forces between molecules also increases. This trend is similar to that observed for alcohols and other compounds described earlier.

Solubility

Solubility in water

Molecules of aldehydes, ketones and esters cannot form hydrogen bonds with each other. However, Figure 13.3.25 shows how hydrogen bonds can form between a lone pair of electrons on the oxygen atom of the carbonyl group and the partially positive hydrogen atoms in water molecules. The strength of this interaction is enough to make small aldehydes, ketones and, to a lesser extent, esters soluble in water.

As for other soluble organic compounds such as alcohols, when the non-polar hydrocarbon chain length of aldehydes, ketones and esters increases, their solubility in water decreases.

Solubility in organic solvents

As the non-polar hydrocarbon chain of aldehydes, ketones and esters increases in length, they become more soluble in non-polar solvents. This is opposite to the trend observed in water.

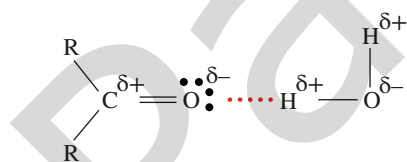


FIGURE 13.3.25 Hydrogen bonds form between the negatively charged electron pair on the oxygen atom in a carbonyl group and the positively charged hydrogen atom in a water molecule.

EXTENSION

Flashpoint

When a candle burns, the solid candle wax must be converted to a vapour before it will ignite. The match used to light the candle first melts some of the wax soaked into the candlewick and vaporises it. It is the wax vapour, rather than the solid candle wax, that ignites and actually burns. Close observation of a burning candle, such as the one shown in Figure 13.3.26, confirms this.



FIGURE 13.3.26 Close observation of a candle shows that it is the candle-wax vapour rather than the solid wax that burns.

Similarly, for liquid fuels such as petrol and methylated spirits, it is the vapour that burns, rather than the liquid. As the temperature of a liquid fuel increases, the concentration of vapour above the surface of the liquid rises. At a certain temperature, there will be enough fuel vapour mixed with the air for the fuel to burn. The temperature at which a vapour ignites is called the flashpoint.

The flashpoint is defined as the lowest temperature at which a liquid forms sufficient vapour to ignite when an ignition source (such as a flame) is applied (Figure 13.3.27). The flashpoints of some common fuels are shown in Table 13.3.5.



TABLE 13.3.5 Flashpoints of some common fuels

Fuel	Flashpoint (°C)
Ethanol	16
Petrol	-43
Diesel	>52
Jet fuel	>38

The flashpoints of hydrocarbon fuels, such as petrol, diesel and kerosene, are related to the boiling points of the fuels. The boiling points of hydrocarbons are a property of the carbon-carbon chain length of the hydrocarbon molecules in the fuels. This trend is also observed when measuring flashpoints (Table 13.3.6).

TABLE 13.3.6 Flashpoints of a selection of alkanes with increasing molecular size

Alkane	Number of carbon atoms in chain	Flashpoint (°C)
Butane	4	-76
Methylpropane	4	-83
Hexane	6	-7
Heptane	7	25
Octane	8	56

The shape of a molecule can also affect a compound's physical properties. Methylpropane and butane are isomers, with a molecular formula of C_4H_{10} . The dispersion forces between methylpropane molecules are weaker than in butane, so methylpropane has a lower boiling point and lower flashpoint than butane.

While the low flashpoints of fuels make them useful in engines, their use also has dangers. That is why when putting petrol in a car, you should not smoke or use a naked flame of any kind. Gas supplies, including bottled gas, have additives with unpleasant odours that make it possible to detect and respond to gas leaks before an explosion occurs.

FIGURE 13.3.27 This apparatus measures the flashpoint of fuels. The fuel is heated steadily in a metal cup and, at intervals, a flame is brought above the liquid in the cup. The flashpoint is the lowest temperature at which the fuel will ignite when the flame is brought above it.

Properties and uses of esters

Esters are compounds that often have characteristic sweet, fruity odours. Many esters occur naturally in fruits and flowers. The distinctive and appealing odour of your favourite perfume or aftershave may well be due to esters.

Although esters are polar, they have no free hydroxyl groups, so they cannot form hydrogen bonds with each other. Therefore, they have lower boiling points than carboxylic acids and alcohols of similar relative molecular mass (Figure 13.3.28).

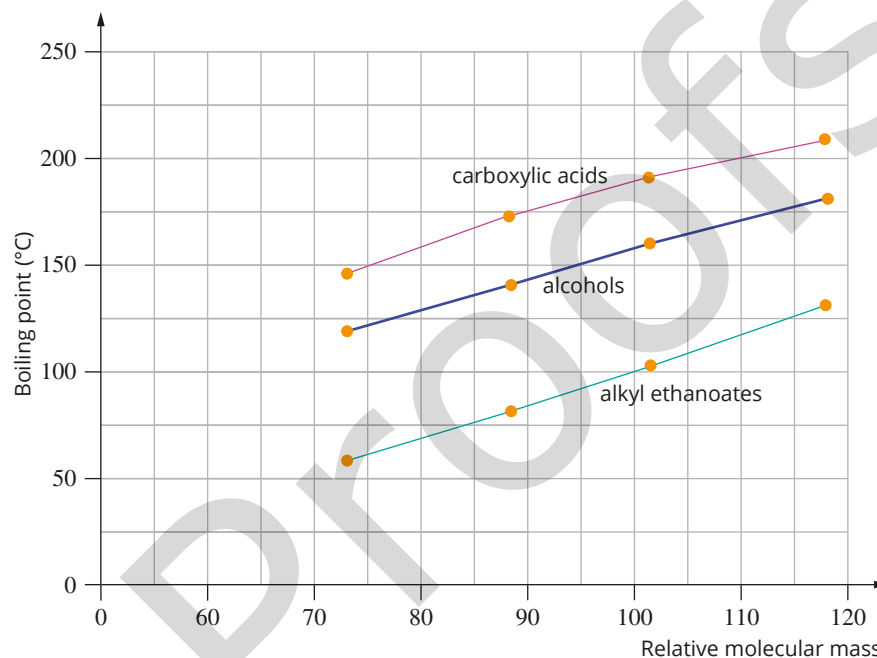


FIGURE 13.3.28 Boiling points of alkyl ethanoates (a series of esters) compared to carboxylic acids and alcohols of similar relative molecular mass.



FIGURE 13.3.29 Beeswax is largely composed of an ester called triacontanyl palmitate.

Smaller esters are liquids at room temperature. They are good solvents for many organic compounds. For example, butyl ethanoate is used as a paint thinner and ethyl ethanoate is found in nail polish removers. Many esters are large molecules and exist as oils and waxes. For example, beeswax is largely composed of an ester called triacontanyl palmitate (Figure 13.3.29).

CHEMFILE

Esters, sweet flavours and strong aromas

Esters are responsible for some of the natural and synthetic flavours and smells found in ice creams, lollies, flowers and fruit (Figure 13.3.30). Table 13.3.7 lists the names of some esters with distinctive smells or flavours.



FIGURE 13.3.30 Esters are responsible for many of the flavours and odours of fruit.

TABLE 13.3.7 Some sweet smelling esters

Ester	Smell or flavour
Pentyl propanoate	Apricot
Ethyl butanoate	Pineapple
Octyl ethanoate	Orange
2-Methylpropyl methanoate	Raspberry
Ethyl methanoate	Rum
Pentyl ethanoate	Banana

13.3 Review

SUMMARY

- The boiling points of organic molecules are determined by intermolecular forces. Dispersion forces are always present and there may also be dipole–dipole attractions or hydrogen bonds.
- The strength of dispersion forces between alkane molecules depends on the size and shape of the molecules.
- The only forces of attraction between molecules of the alkane and alkene homologous series are dispersion forces.
- Molecules of aldehydes, ketones and esters have polar carbonyl functional groups and they are attracted to each other by dipole–dipole attractions.
- Molecules of alcohols, carboxylic acids, amines and amides contain functional groups that can form hydrogen bonds with other molecules.
- Comparing molecules of similar size in different homologous series, it is generally true that their boiling points increase in the order: alkanes, alkenes < aldehydes, ketones, esters < alcohols, carboxylic acids, amines, amides.
- The solubility of organic molecules in water is determined by the way the water molecules interact with the molecules of the solvent. This is affected by the polarity of functional groups and the length of the non-polar hydrocarbon tails.
- Alkanes and alkenes are insoluble in water.
- The smaller members of the aldehyde, ketone, ester, alcohol, amine and amide homologous series are generally soluble in water. Solubility rapidly decreases as the chain length increases.
- Alkanes and alkenes are soluble in non-polar organic solvents.
- The solubility of aldehydes, ketones, esters, alcohols, amines and amides in non-polar organic solvents increases as the chain length of the molecules increases.

KEY QUESTIONS

- 1 Complete the following paragraph by filling in the gaps with the appropriate words.
Butane is a member of the _____ homologous series. The forces of attraction holding butane molecules to each other are _____. As the chain length of alkanes increases, their boiling points _____. Alkanes are _____ in water. This is because the forces of attraction between water molecules and alkane molecules are _____ than the _____ between water molecules.
- 2 Arrange the following compounds in increasing order of boiling point. Provide reasons for your answer.
 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$, $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_3$,
 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$,
 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$
- 3 Arrange the following compounds in increasing order of boiling point.
 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$, CH_3CH , CH_3CHCH_2 , $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$,
 $\text{CH}_3\text{CH}_2\text{CH}_2\text{COOH}$

13.4 Isomers overview

Isomers are molecules that contain the same number and type of atoms, arranged in different ways. The existence of isomers is a major reason why there are so many different carbon compounds. Isomers have the same molecular formula but they can have different physical and chemical properties and so behave differently.

There are two main types of isomers considered in this course:

- **structural (positional and chain) isomers**
- **geometric (*cis-trans*) isomers.**

Structural isomers form when the atoms in molecules with the same molecular formula bond together in different arrangements. Two types of structural isomers are **chain isomers** and **positional isomers**.

CHAIN ISOMERS

Chain isomers form because of the branching that is possible in the carbon chains that form the backbone of any large organic molecule. Chain isomers of alkanes can contain more than one **alkyl group**; some molecules may also have more than one alkyl group attached to the same carbon atom.

Hexane is an example of an alkane with no branches. It has the molecular formula C_6H_{14} and its structure is shown in Figure 13.4.1.

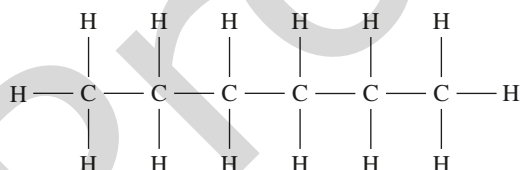


FIGURE 13.4.1 Hexane is a single-chain hydrocarbon with single bonds that contains six carbon atoms and fourteen hydrogen atoms.

Three of the chain isomers of hexane are shown in Figure 13.4.2. Each isomer has a different name that represents its exact molecular structure. The naming of chain isomers is described in the next section.

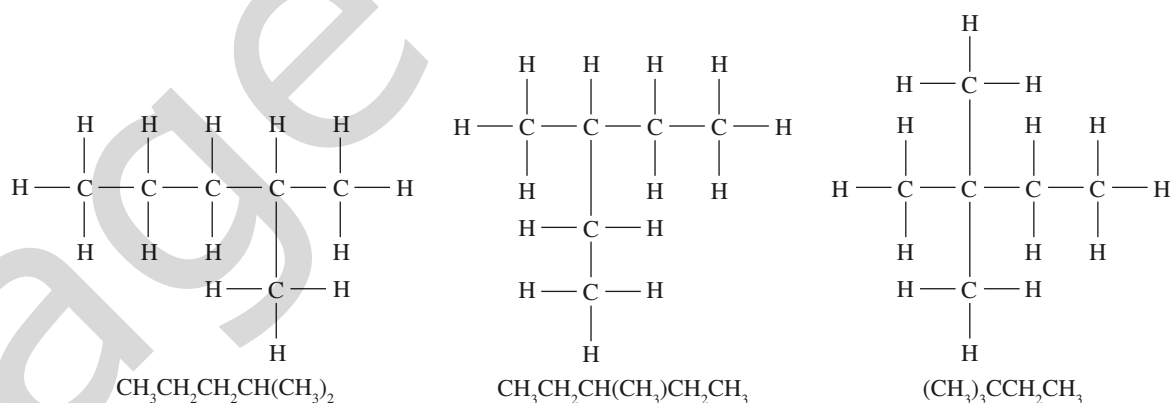


FIGURE 13.4.2 Three chain isomers of hexane

POSITIONAL ISOMERS

Positional isomers can occur for organic molecules that contain functional groups. Two molecules with the same carbon chain and functional group but with the functional group in a different location in the molecule are called positional isomers.

Alcohols are organic molecules that contain a hydroxyl ($-OH$) functional group. A number of positional isomers can be drawn for an alcohol with the molecular formula $C_4H_{10}O$. Like chain isomers, each positional isomer is given a different name. Figure 13.4.3 shows two positional isomers, butan-1-ol and butan-2-ol.

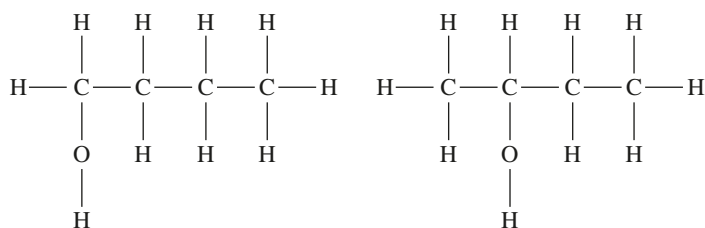


FIGURE 13.4.3 Two positional isomers of an alcohol with the formula $\text{C}_4\text{H}_{10}\text{O}$

It is important to realise that alkenes also contain functional groups—their double carbon–carbon bonds. This means that positional isomers can be formed when the double bond is in different locations. Figure 13.4.4 shows the two positional isomers of butene.

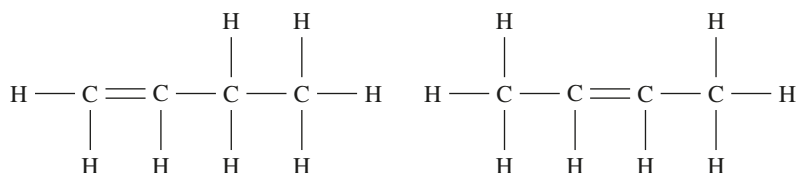


FIGURE 13.4.4 The two positional isomers of butene: but-1-ene and but-2-ene

Positional isomers only exist for molecules that contain a functional group and have a long enough carbon chain that different positions of the functional group are possible. When drawing positional isomers, be careful that you do not just draw the same molecule from a different perspective. You can see that the two structural formulae of ethanol in Figure 13.4.5 do not represent positional isomers.

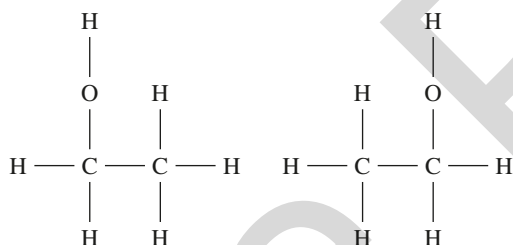


FIGURE 13.4.5 Two representations of the structure of ethanol ($\text{C}_2\text{H}_6\text{O}$). These are not positional isomers; if the first structure is flipped over, it is identical to the second.

It is possible for structural isomers to form both positional and chain isomers. Figure 13.4.6 shows two more isomers of an alcohol with the formula $\text{C}_4\text{H}_{10}\text{O}$. They are chain isomers of the molecules shown previously in Figure 13.4.5, and positional isomers of each other.

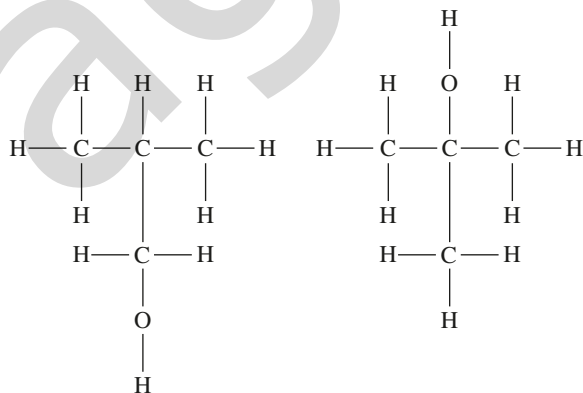


FIGURE 13.4.6 Two more molecules that are alcohols with the molecular formula $\text{C}_4\text{H}_{10}\text{O}$

GEOMETRIC (*CIS-TRANS*) ISOMERS

Geometric isomers can occur when there is restricted rotation somewhere in a molecule. Restricted rotation can occur about a carbon–carbon double bond or within a ring.

Two atoms joined by a single bond can rotate freely around the single bond. You might think that the two models shown in Figure 13.4.7 show different molecules, but they are models of the same molecule because there is free rotation around the single bond. The first structure can rotate around the central single bond to look exactly the same as the second molecule.

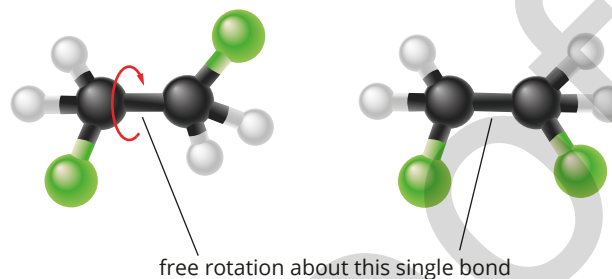


FIGURE 13.4.7 These two models represent the same molecule because the groups on either end can rotate around the single bond.

However, because of the way that the electrons are arranged in a double bond, groups attached to carbons on either side are unable to rotate freely. The models in Figure 13.4.8 represent two molecules that cannot be rotated to form the same structure because a double bond is present.

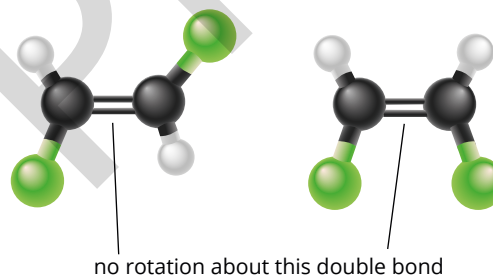


FIGURE 13.4.8 These two models represent different molecules because the groups on either end cannot rotate around the double bond.

cis-trans isomers can occur when there are two different groups attached to each carbon atom involved in the double bond. The different groups can be functional groups or hydrocarbon chains of different lengths. There are two possible arrangements: the groups can be on the same or opposite sides of the double bond. If the groups are on the same side, the isomer is called the ***cis* isomer**. If the groups are on opposite sides, the isomer is called the ***trans* isomer**.

Figure 13.4.9 shows the three possible structures of dibromoethene ($C_2H_2Br_2$). If both bromine atoms are attached to the first carbon atom, then it is called 1,1-dibromoethene. This molecule does not have geometric isomers. If the bromine atoms are attached to different carbon atoms, then it is called 1,2-dibromoethene, which has the condensed structural formula $BrCH=CHBr$. There are two isomers that may form: *cis*-1,2-dibromoethene and *trans*-1,2-dibromoethene.

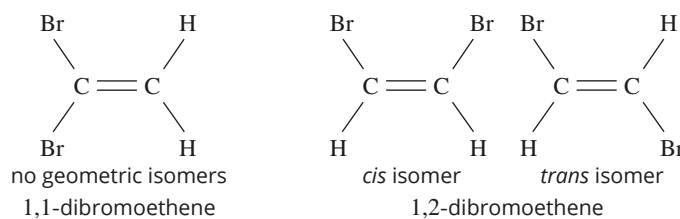


FIGURE 13.4.9 The possible structures of dibromoethene ($C_2H_2Br_2$). Note the position of the bromine atoms in the *cis* and *trans* isomers.

When considering longer alkenes, it is the longest alkyl groups attached to the carbon atoms in the double bond that are used to decide if the molecule is a *cis* or *trans* isomer.

- In *cis* isomers, the longest alkyl groups on each carbon are located on the same side of the double bond.
- In *trans* isomers, the longest alkyl groups on each carbon are located on opposite sides of the double bond.

Figure 13.4.10 shows the *cis* and *trans* isomers of but-2-ene.

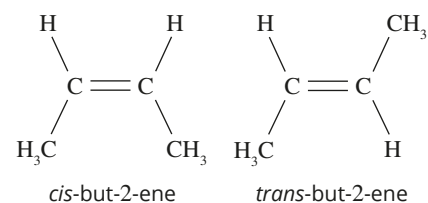


FIGURE 13.4.10 The two isomers of but-2-ene both have the condensed structural formula $\text{CH}_3\text{CH}=\text{CHCH}_3$. The two methyl groups are on the same side of the double bond in the *cis* isomer. The methyl groups are opposite each other in the *trans* isomer.

CHEMISTRY IN ACTION

The correlation between *trans*-fatty acids and coronary heart disease

Trans-fatty acids occur in small amounts in nature but are also produced from vegetable oils for use in many common foods such as margarine and the frying of fast foods. *Trans*-fatty acids are hydrocarbon chains with a *trans* carbon-carbon double bond. This means the fatty acid chains pack together quite tightly (as opposed to *cis*-isomers). This tight packing gives them more desirable melting and boiling points.

In recent years, studies have shown there has been a correlation between the intake of *trans*-fatty acids in the diet and the risk of coronary heart disease. Coronary heart disease results when the coronary arteries get narrower, restricting the flow of blood to the heart. This narrowing is caused by fatty material (cholesterol) that gradually builds up inside the arteries. The recommendation from The Heart Foundation is that less than 1% of total energy should come from *trans*-fats.

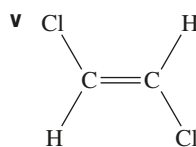
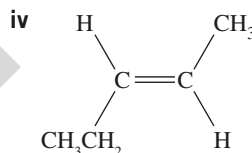
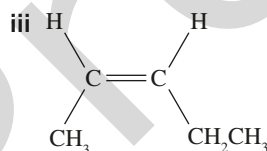
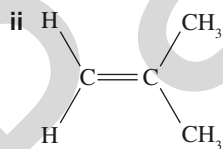
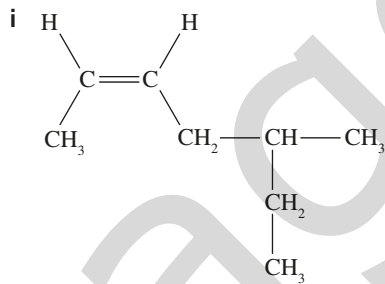
13.4 Review

SUMMARY

- Carbon compounds can have structural isomers and geometric (*cis-trans*) isomers. Structural isomers include chain and positional isomers.
- Chain isomers have the same molecular formula but different branching of the carbon chain.
- Positional isomers have the same molecular formula but at least one functional group in different positions on the carbon chain.
- Geometric (*cis-trans*) isomers occur when there is restricted rotation somewhere in a molecule. Restricted rotation can occur about a carbon-carbon double bond or a ring.
- *cis-trans* isomers are geometric isomers of alkenes that occur when there are two different groups attached to the carbon atoms at each end of a carbon-carbon double bond.
- In *cis-trans* isomers of alkenes, the atoms in the isomers are joined in the same order, but have a different arrangement in space

KEY QUESTIONS

- a Which is the shortest alkane that can have chain isomers?
 - b Draw structural formulae for all the chain isomers of this alkane.
- 2 Explain why carbon chains in alkanes are not straight as commonly drawn in structural formulae.
- 3 Look at the following alkenes.
 - a Which alkenes have *cis-trans* isomers?
 - b Which alkenes are *cis* isomers?
 - c Which alkenes do not have *cis-trans* isomers? Explain why.



13.5 IUPAC nomenclature overview

In the early 1960s, IUPAC endorsed a common naming system for carbon compounds. These rules are regularly updated and are used worldwide to enable scientists to communicate with each other. The rules ensure that a carbon compound is given a unique name that provides useful information about its structure and distinguishes it from any isomers.

The rules specify the names for different parts of an organic molecule and may include both words and numbers to indicate locations of functional groups and alkyl branches (for example, see Figure 13.5.1).

This section will summarise and extend your knowledge of the rules that you learnt in the previous sections for naming organic compounds. You will also learn how to name organic molecules that contain two different functional groups.

IUPAC NOMENCLATURE

IUPAC nomenclature is the set of rules by which chemists can name a given compound. The rules can be used in reverse to derive a structure from the IUPAC name. IUPAC names of organic molecules can be simple or complex, but most IUPAC names follow the same basic pattern.

All organic molecules can be thought of as being derived from a hydrocarbon parent molecule, which provides the basis for the name of the molecule. Part of the IUPAC name reflects which alkane is the parent molecule.

The IUPAC name also indicates which functional groups are present in the molecule by adding a suffix to the end of the name or a prefix to the beginning of the name. The positions of functional groups are indicated by numbers. As an example, the meaning of each part of the name butan-2-ol, an alcohol, is shown in Figure 13.5.2 along with its structural formula.

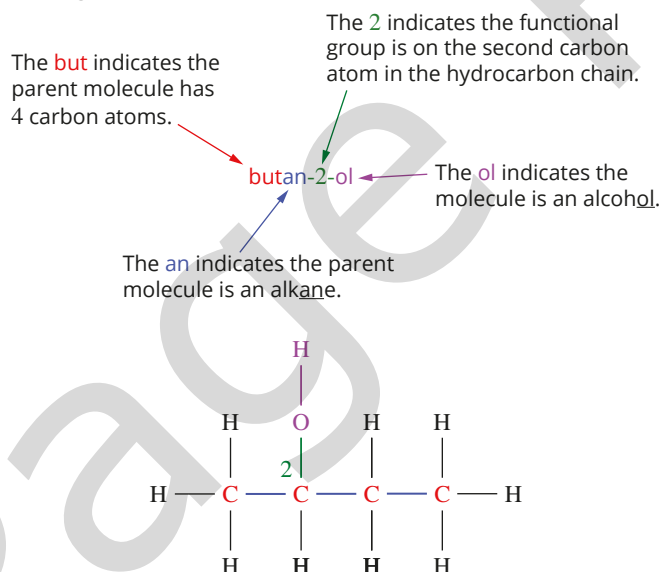


FIGURE 13.5.2 The name and structural formula of butan-2-ol. The colours of each part of the name correspond with the section of the structure that it represents.

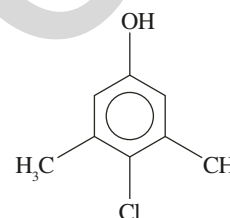


FIGURE 13.5.1 According to the IUPAC rules, the active ingredient in the antiseptic Dettol has the name 4-chloro-3,5-dimethylphenol.

SUMMARY OF IUPAC RULES FOR NOMENCLATURE

The following conventions are used for naming organic molecules.

- The longest carbon chain is used to derive the parent name. The longest chain must include the functional group for alkenes, alcohols, amines, carboxylic acids and esters.
- The names and locations of branches and additional functional groups are added to this parent name.
- Numbers are used to identify the carbon atom that groups are attached to.
- Numbers and letters are separated by hyphens.
- Numbers are separated from other numbers by commas.
- There are no spaces in a name, apart from the two-word names of acids and esters.
- The names of branching alkyl groups are added before the parent name.
- If there is more than one type of functional group to be listed at the beginning of a name, they are listed in alphabetical order.
- If there is more than one of the same type of functional group, the prefixes 'di-', 'tri-' or 'tetra-' are used. Each group is still given a number to indicate its position on the carbon chain.

The presence of a particular functional group identifies the homologous series a molecule belongs to and changes the molecule's name, as shown in Table 13.5.1.

TABLE 13.5.1 The identity, functional groups and naming conventions of the homologous series

Homologous series	Functional group name	Condensed structural formula	Naming convention
Alkane	Not applicable	Not applicable	Suffix -ane
Alkene	Carbon-carbon double bond	-C=C-	Suffix -ene
Haloalkane	Halo	-F, -Cl, -Br, -I	Prefix fluoro-, chloro-, bromo- or iodo-
Alcohol	Hydroxyl	-OH	Suffix -ol Occasionally prefix hydroxy-
Amine	Amino	-NH ₂	Suffix -amine Occasionally prefix amino-
Carboxylic acid	Carboxyl	-COOH	Suffix -oic acid
Ester	Ester	-COO-	Two-word name with suffixes -yl and -oate
Aldehyde	Carbonyl (end of carbon chain)	-CHO	Suffix -al
Ketone	Carbonyl (within carbon chain)	-CO-	Suffix -one
Amide	Amide	-CONH ₂	Suffix -amide

Naming organic molecules with a functional group and alkyl side chain

Organic molecules with functional groups can also have alkyl side chains. The names of alkyl groups are placed in alphabetical order in front of the parent name. The carbon chain is numbered from the end closest to the functional group to give the lowest possible number to the functional group.

This procedure is illustrated in Table 13.5.2 with the naming of the structural isomers of an alcohol with the molecular formula $C_4H_{10}O$.

TABLE 13.5.2 Names of isomers of an alcohol with the molecular formula $C_4H_{10}O$

Structure	Name
$\begin{array}{ccccccc} & \text{H} & \text{H} & \text{H} & \text{H} & & \\ & & & & & & \\ \text{H} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{O} & - \text{H} \\ & & & & & & \\ & \text{H} & \text{H} & \text{H} & \text{H} & & \end{array}$	Butan-1-ol
$\begin{array}{ccccccc} & & & \text{H} & & & \\ & & & & & & \\ & \text{H} & \text{H} & \text{O} & \text{H} & & \\ & & & & & & \\ \text{H} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{H} \\ & & & & & & \\ & \text{H} & \text{H} & \text{H} & \text{H} & & \end{array}$	Butan-2-ol
$\begin{array}{ccccccc} & & & \text{H} & & & \\ & & & & & & \\ & \text{H} & - \text{C} & - \text{H} & & & \\ & & & & & & \\ & \text{H} & & \text{H} & & & \\ \text{H} & - \text{C} & - \text{C} & - \text{C} & - \text{O} & - \text{H} \\ & & & & & & \\ & \text{H} & \text{H} & \text{H} & & & \end{array}$	2-Methylpropan-1-ol
$\begin{array}{ccccccc} & & & \text{H} & & & \\ & & & & & & \\ & \text{H} & - \text{C} & - \text{H} & & & \\ & & & & & & \\ & \text{H} & & \text{H} & & & \\ \text{H} & - \text{C} & - \text{C} & - \text{C} & - \text{H} \\ & & & & & & \\ & \text{H} & \text{O} & \text{H} & & & \\ & & & & & & \\ & & \text{H} & & & & \end{array}$	2-Methylpropan-2-ol

EXTENSION

Naming organic molecules with two functional groups

Many organic molecules have more than one functional group. If the functional groups are the same, a multiplier (di-, tri- etc.) can be used. If the molecule has different functional groups, you will need to know which one has the highest priority in order to work out what numbers and names to use.

IUPAC has designated a priority system for functional groups (Table 13.5.3). In an organic molecule with two functional groups, the following naming conventions are used.

- The functional group with the highest priority is assigned the lowest possible number and the suffix for this functional group is used in the name.
- The lower priority functional group is indicated by a prefix or alternative name.

TABLE 13.5.3 IUPAC functional group priorities

	Functional group	Suffix	Alternative name (when needed)
Highest priority	Carboxyl	-oic acid	–
↓	Hydroxyl	-ol	hydroxy-
	Amino	-amine	amino-
	Alkene	-ene	-an- becomes -en-
Lowest priority	Halo	–	halo-

This priority system is illustrated in Table 13.5.4 with the naming of molecules with two functional groups.

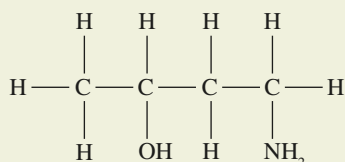
TABLE 13.5.4 Naming molecules with two functional groups

Structure	Name
$ \begin{array}{ccccccc} & \text{H} & \text{H} & \text{H} & \text{O} & & \\ & & & & & & \\ \text{H} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{O} & - \text{H} \\ & & & & & & \\ & \text{H} & \text{O} & \text{H} & & & \\ & & & & & & \\ & & \text{H} & & & & \end{array} $	3-Hydroxybutanoic acid
$ \begin{array}{ccccccc} & & \text{H} & & \text{H} & & \\ & & & & & & \\ \text{H} & - \text{O} & - \text{C} & - \text{C} & - \text{N} & - \text{H} & \\ & & & & & & \\ & & \text{H} & & \text{H} & & \end{array} $	2-Aminoethanol
$ \begin{array}{ccccccc} & \text{H} & \text{H} & \text{H} & \text{H} & \text{Cl} & \\ & & & & & & \\ \text{H} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{C} & - \text{H} \\ & & & & & & \\ & \text{H} & \text{O} & \text{H} & \text{H} & \text{H} & \\ & & & & & & \\ & & \text{H} & & & & \end{array} $	5-Chloropentan-2-ol

Worked example 13.5.1

NAMING AN ORGANIC MOLECULE WITH TWO FUNCTIONAL GROUPS

Name this molecule according to IUPAC rules.

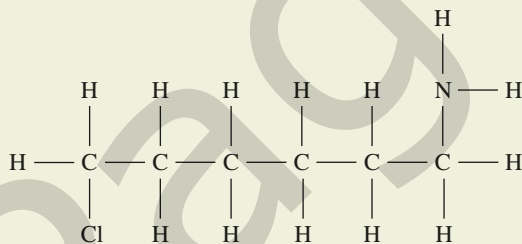


Thinking	Working
Identify the parent name by counting the longest continuous chain of carbon atoms.	There are four carbons in the longest chain, so the parent name is butane.
Identify the functional groups present.	The two functional groups present are hydroxyl and amino.
Determine which functional group has the higher priority and determine the prefixes and suffixes to use.	The hydroxyl group has the higher priority, so the molecule will end in -ol. The amino group has lower priority and so the prefix amino- will be used.
Number the carbon chain, giving the highest priority group the lowest number possible.	$\begin{array}{cccc} \text{H} & \text{H} & \text{H} & \text{H} \\ & & & \\ \text{H}-\text{C} & -\text{C} & -\text{C} & -\text{C}-\text{H} \\ & & & \\ \text{H} & \text{OH} & \text{H} & \text{NH}_2 \end{array}$ The numbers 1, 2, 3, and 4 are placed above the first, second, third, and fourth carbon atoms respectively.
Determine the number of the carbon each functional group is attached to.	The -OH is attached to carbon 2 and -NH ₂ is attached to carbon 4.
Use the functional group names and carbon numbers to construct the full name.	The name of the molecule is 4-aminobutan-2-ol.

Worked example: Try yourself 13.5.1

NAMING AN ORGANIC MOLECULE WITH TWO FUNCTIONAL GROUPS

Name this molecule according to IUPAC rules.

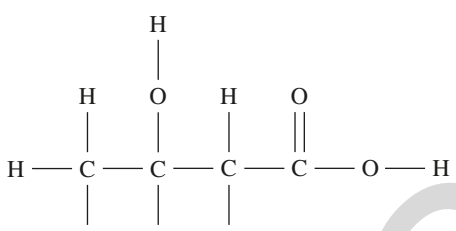
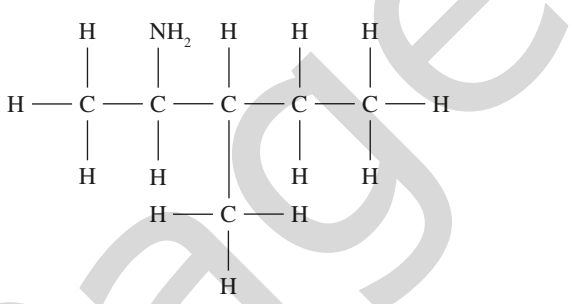


13.5 Review

SUMMARY

- IUPAC nomenclature is a set of rules for naming an organic compound.
- The naming of organic molecules follows a series of steps.
 - Identify the longest unbranched carbon chain to determine the parent name.
 - Name functional groups by prefixes or suffixes.
- Number the carbon chain so that the carbon attached to the highest priority functional group has the lowest number.
- Insert numbers before each functional group.
- When multiples of a functional group are present, use a multiplier (e.g. 'di-').

KEY QUESTIONS

- 1 Draw the structural formula of the functional group of each of the following homologous series.
 - a Carboxylic acid
 - b Aldehyde
 - c Amide
 - d Alcohol
 - e Ester
- 2 Write the systematic name for the following molecules.
 - a 
 - b 
- 3 Draw the structure of:
 - a 2-methylpropan-1-ol
 - b butan-2-ol
 - c 3,4-diethylhex-3-ene.
- 4
 - a Write the condensed formulae based on the following incorrect names.
 - i 3-Aminopropane
 - ii 3-Ethyl-hydroxy-2-butane
 - b Explain why each name is incorrect and give the correct name.

13.6 Determining formulae of organic compounds

When chemists determine the structure of a new compound, one of the most useful pieces of information is the chemical formula of the compound. Even large chemical compounds have a chemical formula. For example, Figure 13.6.1 shows the structure of the hormone insulin, which has a chemical formula of $C_{257}H_{383}N_{65}O_{77}S_6$.

Insulin is a hormone responsible for regulating sugar levels in the body. Determining the formula was a very important step in working out the structure of insulin. Once the formula of insulin was established, scientists were able to carry out research on chemical reactions that could influence the way it operates in the body.

In this section, you will learn about ways in which the chemical formulae of compounds can be determined.

CALCULATING PERCENTAGE COMPOSITION OF ORGANIC COMPOUNDS

The **percentage composition** of a compound tells you the proportion by mass of the different elements in that compound.

To determine the percentage composition by mass of a compound, divide the mass of each element present by the mass of the whole sample and express the result as a percentage.

$$\% \text{ by mass of an element in a compound} = \frac{\text{mass of the element present}}{\text{total mass of the compound}} \times 100$$

Worked example 13.6.1

CALCULATING PERCENTAGE COMPOSITION OF ORGANIC COMPOUNDS

2.85 g of an organic compound contains 1.52 g carbon, 0.45 g hydrogen and 0.88 g nitrogen. Determine the percentage composition of the compound.

Thinking	Working
Divide the mass of the first element by the total mass of the compound and multiply by 100.	$\begin{aligned} \% \text{ carbon} &= \frac{\text{mass of carbon present}}{\text{total mass of the compound}} \times 100 \\ &= \frac{1.52}{2.85} \times 100 \\ &= 53.3\% \end{aligned}$
Divide the mass of the second element by the total mass of the compound and multiply by 100.	$\begin{aligned} \% \text{ hydrogen} &= \frac{\text{mass of hydrogen present}}{\text{total mass of the compound}} \times 100 \\ &= \frac{0.45}{2.85} \times 100 \\ &= 15.8\% \end{aligned}$
Repeat the previous step for any further elements in the compound.	$\begin{aligned} \% \text{ nitrogen} &= \frac{\text{mass of nitrogen present}}{\text{total mass of the compound}} \times 100 \\ &= \frac{0.88}{2.85} \times 100 \\ &= 30.9\% \end{aligned}$
Add up all the elemental percentages to check that they equal 100%. (If they don't, then check your calculations and rounding off.)	$\begin{aligned} \text{If the calculations above are correct, then} \\ \text{Total \% elements} &= \% \text{ carbon} + \% \text{ hydrogen} \\ &\quad + \% \text{ nitrogen} \\ &= 53.3 + 15.8 + 30.9 \\ &= 100\% \end{aligned}$



FIGURE 13.6.1 A representation of the chemical structure of the hormone insulin

Worked example: Try yourself 13.6.1

CALCULATING PERCENTAGE COMPOSITION OF ORGANIC COMPOUNDS

8.38 g of an organic compound contains 5.44 g carbon, 1.13 g hydrogen and 1.81 g oxygen. Determine the percentage composition of the compound. Give all answers to three significant figures.

USING PERCENTAGE COMPOSITION TO DETERMINE EMPIRICAL FORMULAE

Empirical formula

Atoms or ions are present in compounds in fixed whole number ratios. The **empirical formula** of a compound gives the simplest whole number ratio of elements in that compound. See Table 13.6.1 for some examples.

TABLE 13.6.1 Empirical formulae for some examples

Compound	Empirical formula	Simplest whole number ratio of elements in the compound
Water	H ₂ O	H : O 2 : 1
Ethene	CH ₂	C : H 1 : 2
Calcium carbonate	CaCO ₃	Ca : C : O 1 : 1 : 3

Determining empirical formulae

The empirical formula for a compound is determined from the mass of each element present in a given mass of the compound. These masses can be determined experimentally. Once the masses of elements in a compound are known, the steps in Figure 13.6.2 are followed to convert these masses to a mole ratio, that is, a ratio by number of atoms, and then to an empirical formula.

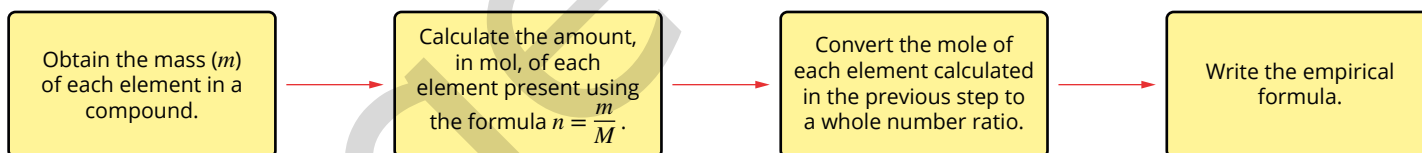


FIGURE 13.6.2 Follow these steps to calculate empirical formula.

Worked Example 13.6.2 shows how to calculate the empirical formula of an unknown organic compound.

Worked example 13.6.2

CALCULATING EMPIRICAL FORMULA FROM PERCENTAGE COMPOSITION

An organic compound is found to be composed of 52.2% carbon, 13.0% hydrogen and the remainder is oxygen. Calculate the empirical formula of the compound.	
Thinking	Working
Assume there is 100 g of the compound, so percentages convert directly to masses. Write down the mass, in g, of all elements present in the compound.	C: 52.2 g H: 13.0 g O: $100 - 52.2 - 13.0 = 34.8$ g
Calculate the amount, in mol, of each element in the compound using: $n = \frac{m}{M}$	$n(\text{C}) = \frac{52.2}{12.0}$ $= 4.35$ $n(\text{H}) = \frac{13.0}{1.0}$ $= 13.0$ $n(\text{O}) = \frac{34.8}{16.0}$ $= 2.18$
Simplify by dividing all of the numbers of moles by the smallest number of moles calculated above. This gives you a ratio of the elements by number of atoms.	$\text{C} = \frac{4.35}{2.18}$ $= 2.0$ $\text{H} = \frac{13.0}{2.18}$ $= 6.0$ $\text{O} = \frac{2.18}{2.18}$ $= 1.0$
Find the simplest whole number ratio.	C : H : O 2 : 6 : 1
Write the empirical formula.	$\text{C}_2\text{H}_6\text{O}$

Worked example: Try yourself 13.6.2

CALCULATING EMPIRICAL FORMULA FROM PERCENTAGE COMPOSITION

Chemical analysis of an organic compound present in the gaseous emissions from a factory shows that its percentage composition is 40.0% carbon, 6.7% hydrogen and the remainder is oxygen. Find its empirical formula.

ELEMENTAL ANALYSIS: MEASURING THE MASS OF EACH ELEMENT IN A COMPOUND

In the examples above, the mass of each element in the sample of the compound was provided. That information comes from an experiment called **elemental analysis**.

One way of performing an elemental analysis of an organic compound is to burn the compound in air. The combustion products, (carbon dioxide and water) are absorbed by chemicals that have been previously weighed to determine the mass of the products produced.

- Carbon dioxide can be absorbed by sodium hydroxide solution.
- Water is absorbed in a drying agent such as magnesium perchlorate ($\text{Mg}(\text{ClO}_4)_2$).

The experimental apparatus is shown in Figure 13.6.3.

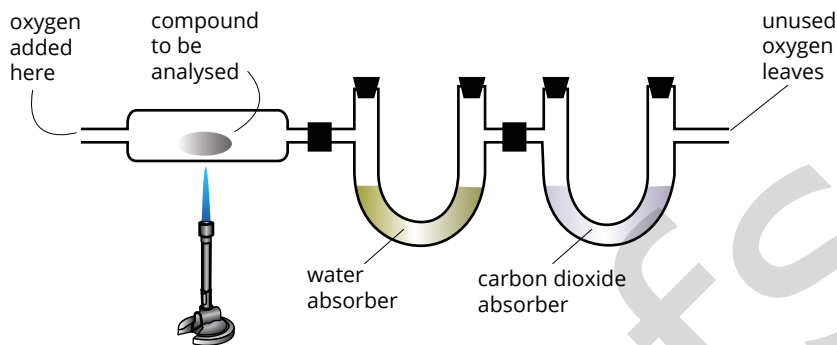


FIGURE 13.6.3 Experimental set-up for the elemental analysis of an organic compound.

The empirical formula of a hydrocarbon or a compound containing only carbon, hydrogen and oxygen can be calculated from the masses of carbon dioxide and water obtained by elemental analysis.

Determining the mass of carbon in the organic compound

Suppose an empirical formula calculation is being carried out on an organic compound containing only carbon, hydrogen and oxygen, using data from elemental analysis. From the mass of carbon dioxide produced, calculate the amount of carbon dioxide produced, in mol:

$$n(\text{CO}_2) = \frac{m}{M} = \frac{m}{44.01}$$

Since all the carbon in the organic compound ends up in the carbon dioxide produced, the amount of carbon dioxide produced, in mol, is equal to the amount of carbon in the organic compound, in mol:

$$n(\text{C}) = n(\text{CO}_2)$$

The mass of carbon in the organic compound can then be determined:

$$m(\text{C}) = n \times M = n \times 12.01$$

Determining the mass of hydrogen in the organic compound

From the mass of water produced, calculate the amount of water produced, in mol:

$$n(\text{H}_2\text{O}) = \frac{m}{M} = \frac{m}{18.016}$$

All the hydrogen in the organic compound ends up in the water produced. The amount of hydrogen in the organic compound, in mol, is twice the amount of water produced, in mol. This is because there are two hydrogen atoms in each molecule of water:

$$n(\text{H}) = 2 \times n(\text{H}_2\text{O})$$

The mass of hydrogen in the organic compound can then be determined:

$$m(\text{H}) = n \times M = n \times 1.008$$

Determining the mass of oxygen in the organic compound

The amount of oxygen in the organic compound cannot simply be determined from the amount of oxygen present in both the carbon dioxide and water produced. This is because the oxygen present in the products comes from two sources—the organic compound and the oxygen gas that was added so that a combustion reaction could occur.

However, the mass of oxygen in the organic compound can be determined by subtracting the mass of carbon plus the mass of hydrogen from the original mass of the compound:

$$m(\text{O}) = m(\text{compound}) - m(\text{C}) - m(\text{H})$$

Once the mass of each element in the organic compound has been determined, the empirical formula can be determined using the steps outlined earlier in this section (Figure 13.6.4).

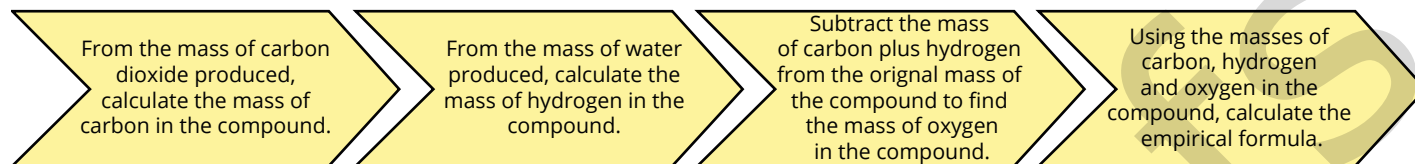


FIGURE 13.6.4 The steps taken to determine the empirical formula from data obtained by elemental analysis

Worked example 13.6.3

CALCULATING THE EMPIRICAL FORMULA OF A COMPOUND

A compound undergoes elemental analysis and was found to contain 12.0g of carbon, 2.0g of hydrogen and 16.0g of oxygen. Determine the empirical formula of the compound.

Thinking	Working
Calculate the number of moles of carbon, hydrogen and oxygen using: $n = \frac{m}{M}$	$n(\text{C}) = \frac{12}{12}$ $= 1.00 \text{ mol}$ $n(\text{H}) = \frac{2.0}{1.00}$ $= 2.00 \text{ mol}$ $n(\text{O}) = \frac{16.0}{16.0}$ $= 1.00 \text{ mol}$
Find the simplest whole number ratio.	C : H : O 1 : 2 : 1
Write the empirical formula.	CH ₂ O

Worked example: Try yourself 13.6.3

CALCULATING THE EMPIRICAL FORMULA OF A COMPOUND

A compound was found to contain 72g of carbon and 18g hydrogen. Determine the empirical formula of the compound.

Determining molecular formulae

The molecular formula of a compound can be determined if you know its empirical formula and its molar mass. Remember that the molar mass of a compound is the mass of one mole of the compound. For example, the molar mass of water (H_2O) is $18.016 \text{ g mol}^{-1}$. Figure 13.6.5 summarises the steps taken to determine the molecular formula from the empirical formula.

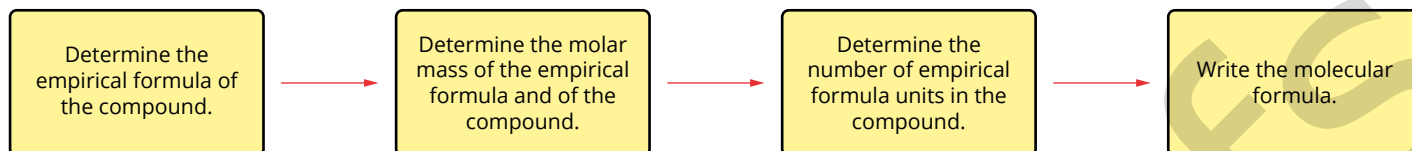


FIGURE 13.6.5 Follow these steps to calculate the molecular formula from the empirical formula.

Worked Example 13.6.4 shows how to calculate a molecular formula.

Worked example 13.6.4

CALCULATING THE MOLECULAR FORMULA OF A COMPOUND

A compound has the empirical formula CH_3 . The molar mass of this compound is 30 g mol^{-1} . What is the molecular formula of the compound?

Thinking	Working
Calculate the molar mass, in g mol^{-1} , of one unit of the empirical formula.	$M(\text{CH}_3) = 12.0 + (3 \times 1.0)$ $= 15.0$
Determine the number of empirical formula units in the molecular formula.	Number of empirical formula units = $\frac{\text{molar mass}}{\text{molar mass of empirical formula unit}}$ $= \frac{30}{15.0}$ $= 2.0$
Multiply the empirical formula by this factor to determine the molecular formula of the compound.	The molecular formula is $2 \times \text{CH}_3$ i.e. C_2H_6

Worked example: Try yourself 13.6.4

CALCULATING THE MOLECULAR FORMULA OF A COMPOUND

A compound has the empirical formula CH . The molar mass of this compound is 78 g mol^{-1} . What is the molecular formula of the compound?

13.6 Review

SUMMARY

- Determining the chemical formula of an unknown compound is an important step in working out its chemical structure.
- The percentage composition of a compound is found by calculating:
$$\frac{\text{mass of the element present}}{\text{total mass of the compound}} \times 100$$
for each element in the compound.
- The empirical formula of a compound can be determined from the percentage composition of each element in the compound.
- The molecular formula of a compound can be determined from its empirical formula and its molar mass.

KEY QUESTIONS

- 1 If 6.84 g of an organic compound is found to contain 4.66 g of carbon, what is the percentage of carbon by mass in the compound?
A 31.8%
B 40.0%
C 60.0%
D 68.1 %
- 2 8.00 g of an organic compound is made up of 6.13 g carbon, 0.51 g hydrogen and the remainder is oxygen. Determine the percentage composition of the compound.
- 3 A clear liquid used for cleaning glass was found to consist of carbon, hydrogen and oxygen. Analysis showed it to be 60.0% carbon and 26.7% oxygen.
 - a Find the mass of each element in 100 g of the compound.
 - b Calculate the number of moles of each element from their masses.
 - c Calculate the simplest mole ratio of each element in the compound. Give your answer to three significant figures.
 - d Give the simplest mole ratio of carbon : oxygen : hydrogen as a whole number ratio.
 - e Write the empirical formula of the compound.
- 4 Mannitol is a sweet-tasting crystalline solid often found in lollies and chewing gum. Its empirical formula is $\text{C}_3\text{H}_7\text{O}_3$. It was determined that 0.8390 mol of mannitol has a mass of 152.7 g. Given this information, determine the molecular formula of mannitol.
- 5 Elemental analysis was conducted on a compound and it was found to contain 72.0 g of carbon, 18.0 g hydrogen and 48.0 g of oxygen. What is the empirical formula of the compound?

Chapter review

KEY TERMS

alcohol	condensation reaction	homologous series	13 S
aldehyde	condensed formula	hydrocarbon	
alkane	crude oil	hydroxyl functional group	
alkene	dimer	immiscible	
alkyl group	dispersion force	isomer	
amide	electronegative	IUPAC nomenclature	
amine	elemental analysis	ketone	
carbonyl functional group	empirical formula	miscible	
carboxyl functional group	ester	molecular formula	
carboxylic acid	ester functional group	organic molecule	
chain isomers	esterification reaction	percentage composition	
<i>cis</i> isomer	fractional distillation	positional isomer	
<i>cis-trans</i> isomers	functional group	primary alcohol	
combustion	geometric isomer	primary amine	
		saturated	
		secondary alcohol	
		semistructural formula	
		stem name	
		structural formula	
		structural isomer	
		tertiary alcohol	
		tetrahedral	
		<i>trans</i> isomer	
		valence shell electron pair	
		repulsion (VSEPR) theory	

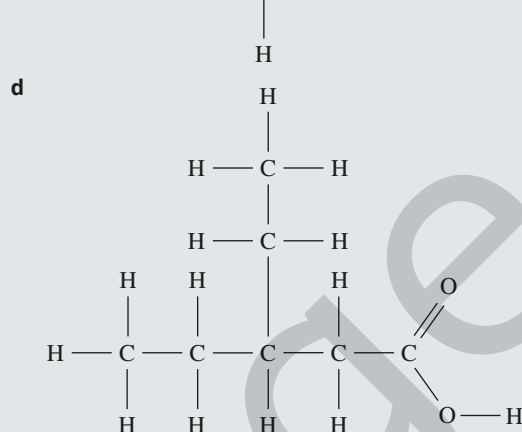
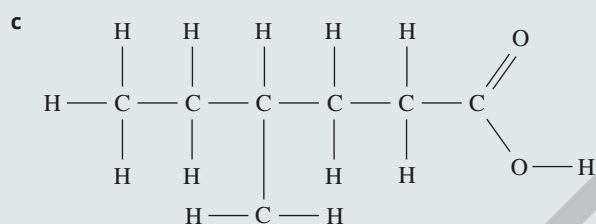
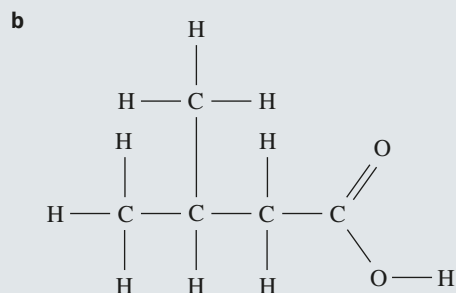
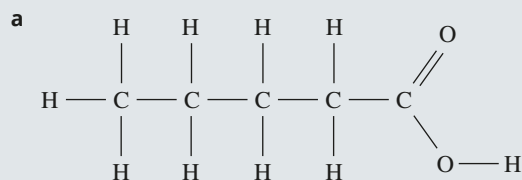
Diversity of carbon compounds

- Why can carbon form so many compounds?
- Which one of the following best describes a homologous series?
 - Compounds in which successive members differ by one carbon and two hydrogen atoms
 - A series of compounds that exist in different physical forms
 - Compounds in which each member differs from the previous one by a $-\text{CH}_3$ group
 - Compounds with the same molecular formula but different arrangements of atoms
- The formula of a hydrocarbon is $\text{C}_{16}\text{H}_{34}$.
 - To which homologous series does it belong?
 - What is the formula of the next hydrocarbon in the homologous series?
 - What is the formula of the previous hydrocarbon in the same homologous series?
 - What mass of carbon is present in 275 g of the hydrocarbon $\text{C}_{16}\text{H}_{34}$?
- Draw the structural formulae and give the systematic names of:
 - CH_3CH_3
 - $\text{CH}_3\text{CH}(\text{CH}_3)_2$
 - $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$
 - $\text{CH}_3(\text{CH}_2)_3\text{CH}_3$
- Draw the structural formulae and give the systematic names of all the isomers of butene.

Functional groups

- Choose the correct response to complete the following sentences to explain why alcohols dissolve in water. An alcohol molecule contains the carboxyl/hydroxyl functional group. This group is non-polar/polar and can form covalent/hydrogen/ionic bonds with water molecules. These intramolecular/intermolecular bonds enable all/large/small alcohol molecules to dissolve in water.
- Identify whether each statement is true or false.
 - A functional group affects the chemical properties of a molecule.
 - The name of the $-\text{OH}$ group in an organic molecule is a hydroxyl functional group.
 - Alcohols contain the carboxyl functional group.
- Which one of the following is a correct condensed structural formula for a carboxylic acid?
 - $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$
 - CH_2CHCH_3
 - $\text{CH}_3\text{COOCH}_3$
 - $\text{CH}_3\text{CH}_2\text{COOH}$
- Two carboxylic acid molecules can bond together to form a dimer. In this dimer, which one of the following is the strongest form of bonding between the two molecules?
 - Hydrogen bonding
 - Dipole-dipole attraction
 - Dispersion forces
 - Carbon-oxygen bonding

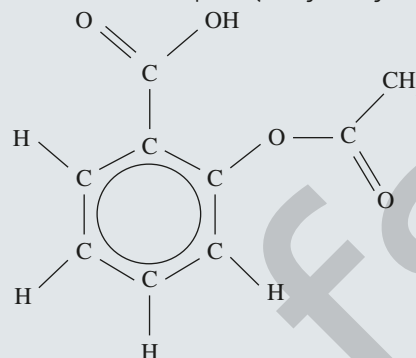
10 Write the systematic names of these carboxylic acids, based on their structural formulae.



11 Draw the structural formulae of the following esters and then name them.

- a $\text{CH}_3\text{COOCH}_3$
 b $\text{CH}_3\text{COOCH}_2\text{CH}_3$
 c $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3$

12 This is the structure of aspirin (acetylsalicylic acid).



- a Identify the ester functional group in the structure of aspirin.
 b Draw the structure of the alcohol and carboxylic acid that reacted together to produce aspirin.

13 What is the structural difference between an aldehyde, a ketone, a carboxylic acid and an amide?

Properties of organic compounds

14 The following table lists the boiling points of the first five alkanes and alcohols (hydroxyl group on carbon number 1).

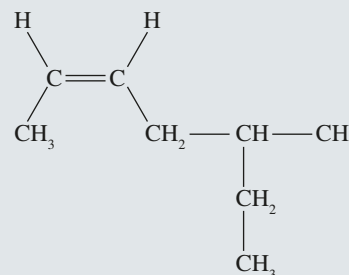
Numbers of carbon atoms	Boiling point of alkane ($^{\circ}\text{C}$)	Boiling point of alcohol ($^{\circ}\text{C}$)
1	-162	65
2	-89	79
3	-42	97
4	0	117
5	36	138

Explain why the alcohols have a higher boiling point than their corresponding alkane.

- 15 Explain why butan-1-ol has a higher boiling point than methanol.
 16 Explain why the solubilities of carboxylic acids in water decrease as the length of their carbon chain increases.

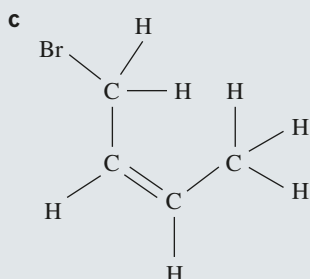
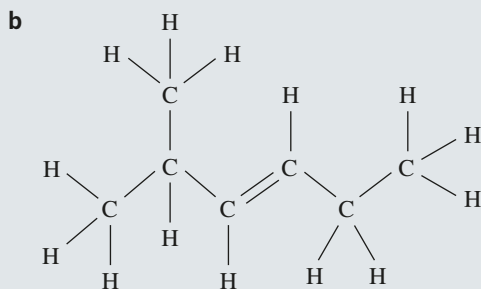
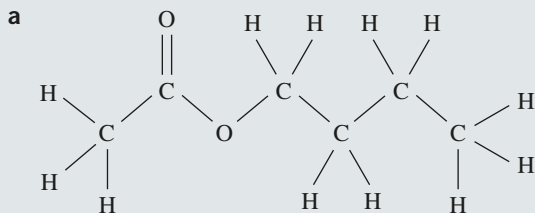
Isomers overview

- 17 Draw the structure of *trans*-methylpent-2-ene.
 18 Write the name of this alkene.



IUPAC nomenclature overview

19 Name each of the following molecules.



20 Draw the structure of:

- heptyl propanoate
- trans*-4-iodo-3-methylpent-2-ene
- 3-methylbutan-1-amine.

Determining formulae of organic compounds

- 21 A sample of an unknown hydrocarbon was found to contain 92.3% carbon by mass. The mass of carbon in the sample was 1.15 g. Determine the mass of hydrogen in the sample.
- 22 Using the empirical formula and the relative molecular mass, determine the molecular formulae of the following compounds.

Empirical formula	Relative molecular mass (g mol^{-1})	Molecular formula
CH	78.0	
CH ₃	30.0	
CH ₂ O	90.0	
C ₃ H ₆ O	116.0	
CH ₂	98.0	

23 A hydrocarbon contains 85.7% carbon and its molar mass is between 40 and 50 g mol^{-1} .

- Calculate the empirical formula of the hydrocarbon.
- Determine its molecular formula.
- To which homologous series does the compound belong?

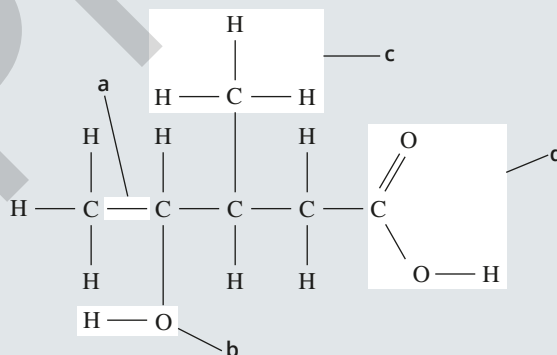
24 An organic compound has the following percentage composition: 40.0% carbon, 6.7% hydrogen and 53.3% oxygen.

- Determine the empirical formula of the organic compound.
- 0.250 mol of this compound has a mass of 15.0 g. Using this information, determine the molecular formula of this organic compound.

25 A 1.50 g sample of a hydrocarbon undergoes complete combustion to produce 4.40 g of carbon dioxide and 2.70 g of water. What is the empirical formula of this compound?

Connecting the main ideas

26 Identify the structures or functional groups labelled a, b, c and d.



- 27 Prepare a poster that summarises the rules for the systematic naming of carbon compounds.
- 28 Explain the following.
- The first member of the alkene homologous series is ethene, not methene.
 - Carbon compounds usually have four covalent bonds around each carbon atom.
- 29 Labels on margarine and oil often include one of the following terms: polyunsaturated, mono-unsaturated, saturated.
- What do you think each of these terms means?
 - Check some food containers at home or in a supermarket and note the details on any labels that include these terms.

30 Explain why each of these names is incorrect, then determine its correct name.

- a But-4-ene
- b 2-Chloro-3-ethylbutane
- c 2,2-Dimethylpent-3-ene
- d 1-Bromo-1,1-dipropylmethane

31 The condensed structural formulae of some organic compounds are given below. For each compound:

- i identify the homologous series to which it belongs
- ii give its systematic name.

- a $\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OH}$
- b $\text{CH}_3(\text{CH}_2)_2\text{CHCl}(\text{CH}_2)_2\text{CH}_3$
- c $\text{CH}_3\text{CHOH}(\text{CH}_2)_3\text{CH}_3$
- d $\text{CH}_3(\text{CH}_2)_3\text{COOH}$
- e $\text{CH}_3\text{CH}_2\text{CHNH}_2\text{CH}_3$
- f $(\text{CH}_3)_2\text{CH}(\text{CH}_2)_5\text{CH}_3$
- g $(\text{CH}_3)_2\text{C}=\text{CH}_2$