SL Paper 3

Benzene is sometimes represented as containing three alternate double and single bonds (Fig.1) and sometimes represented as a hexagon with a circle in the middle (Fig.2).

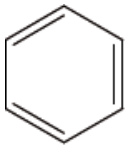


Fig.1

Fig.2

a. Describe two different types of physical evidence which show that benzene does not contain three double bonds. [2]

b. Explain how the reaction of benzene with bromine provides chemical evidence that benzene does not contain three double bonds. [1]

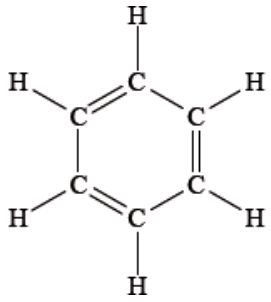
(a) Describe the structure of benzene, C_6H_6.

(b) State **two** pieces of evidence that support this description.

Hydrolysis of aliphatic and aromatic halides occurs under different conditions.

State an equation, using structural formulas, to show the reaction of 1-chloro-2-(chloromethyl) benzene with excess sodium hydroxide at room temperature.

The structure of benzene originally described by August Kekulé is shown below.



Explain, giving **two** different pieces of evidence, why this is not a valid structure for the bonding in benzene.

Following the initial discovery of benzene by Michael Faraday in 1825, it took many years before the structure was determined.

a. Describe the structure of benzene. [3]

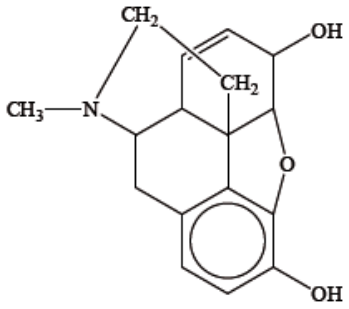
b. State **one** piece of **chemical** evidence proving benzene does not contain alternate single and double bonds. [1]

Analgesics are used to relieve pain in the body. Aspirin and paracetamol (acetaminophen) are both mild analgesics.

The structures of the strong analgesics morphine and heroin (diamorphine) can be found in Table 20 of the Data Book

b. Compare how mild and strong analgesics relieve pain in the body. [2]

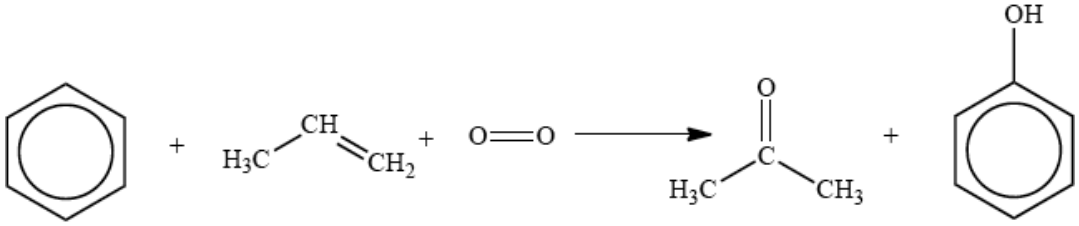
c.i. Identify the amine functional group in the morphine molecule below by drawing a ring around it. [1]



c.iiiState the name of the functional group found in heroin but not in morphine. [1]

d. State **one** advantage and **one** disadvantage of using morphine as a strong analgesic. [2]

The cumene process is used for the production of both propanone and phenol. The overall reaction is shown in the equation below.



This process is important in the polymer industry. Propanone can be converted into methyl methacrylate, the monomer used to make Perspex®, and phenol is used in phenol-methanal resins, which are important thermosetting plastics.

a.ii.State and explain how the presence of a halogen substituent might affect the acidity of carboxylic acids. [3]

d. Propanone could also be formed from propene by reaction with steam over an acidic catalyst, followed by oxidation of the product. [3]

The reaction of propene with water can yield two possible products. Explain, in terms of the stability of the intermediate carbocations, why one is formed in much greater quantities than the other.

Oseltamivir (Tamiflu) and zanamivir (Relenza) are both used as antivirals to help prevent the spread of the flu virus, but are administered by different methods.

a. Zanamivir must be taken by inhalation, not orally. Deduce what this suggests about the bioavailability of zanamivir if taken orally. [1]

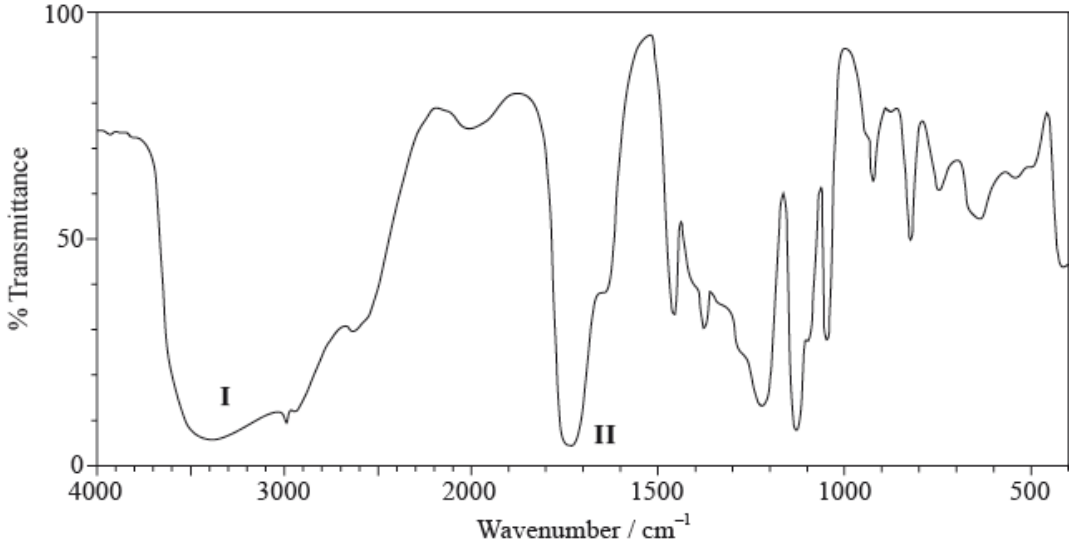
b. Oseltamivir does not possess the carboxyl group needed for activity until it is chemically changed in the body. Deduce the name of the functional group in oseltamivir which changes into a carboxyl group in the body. Use section 37 of the data booklet. [1]

c. The synthesis of oseltamivir is dependent on a supply of the precursor shikimic acid, which is available only in low yield from certain plants, notably Chinese star anise. State one alternative green chemistry source of shikimic acid. [1]

Compound **X** has the molecular formula $C_3H_6O_3$ and is found in human perspiration.

Y is an isomer of **X**, which contains the same functional groups.

a. Its infrared (IR) spectrum is represented below. [1]



[Source: SDBS web: www.sdbs.riodb.aist.go.jp (National Institute of Advanced Industrial Science and Technology, 2013)]

Deduce the bonds responsible for the absorptions labelled **I** and **II**.

I:

II:

b. The $^1H\,NMR$ spectrum recorded showed four peaks with the following chemical shift values (in ppm): [1]

Peaks	Chemical shift / ppm
A	12.4
B	4.0
C	3.4
D	1.2

The integration trace for A:B:C:D was found to be 1:1:1:3.

Deduce what information can be obtained about the hydrogen atoms responsible for peak D at 1.2 ppm from the integration trace in the $^1\mathrm{H\,NMR}$ spectrum of **X**.

c. Deduce the fragments in the mass spectrum which correspond to the following *m/z* values. [2]

m/z = 45:

m/z = 17:

m/z = 15:

d. Deduce the structural formula of **X**. [1]

e. (i) Deduce the structural formula of **Y**. [2]

(ii) Predict **one** difference between the $^1\mathrm{H\,NMR}$ spectrum of **Y** and **X**.

f. (i) Like **X**, 3-methylbutanoic acid is also a source of body odour. Deduce the *m/z* value for the molecular ion peak on the mass spectrum of this compound. [2]

(ii) Deduce the number of different chemical environments of the hydrogen atoms in the $^1\mathrm{H\,NMR}$ spectrum of 3-methylbutanoic acid.

Ethanol is a depressant that is widely consumed in many societies. When consumed excessively it has a major impact on families and society as a whole. Other depressants such as diazepam (Valium®) may be prescribed by a doctor.

One problem associated with ethanol consumption is an increased risk of traffic accidents. Police in many countries use a breathalyser to test drivers. The breathalyser contains potassium dichromate(VI).

b.i. Describe the colour change of potassium dichromate(VI) when it reacts with ethanol. [1]

b.ii. State with a reason whether chromium in potassium dichromate(VI) is oxidised or reduced by ethanol. [1]

Fats and oils have some similarities and some differences in their chemical structures.

a. State **two** major differences in their structures. [2]

b. Describe how an oil can be converted into a fat. [2]

c. Discuss **two** advantages and **two** disadvantages of converting oils into fats. [4]

Alkenes can undergo electrophilic addition reactions with bromine and with hydrogen bromide.

Name the product formed when but-2-ene reacts with

a. Explain how a bromine molecule is able to act as an electrophile. [1]

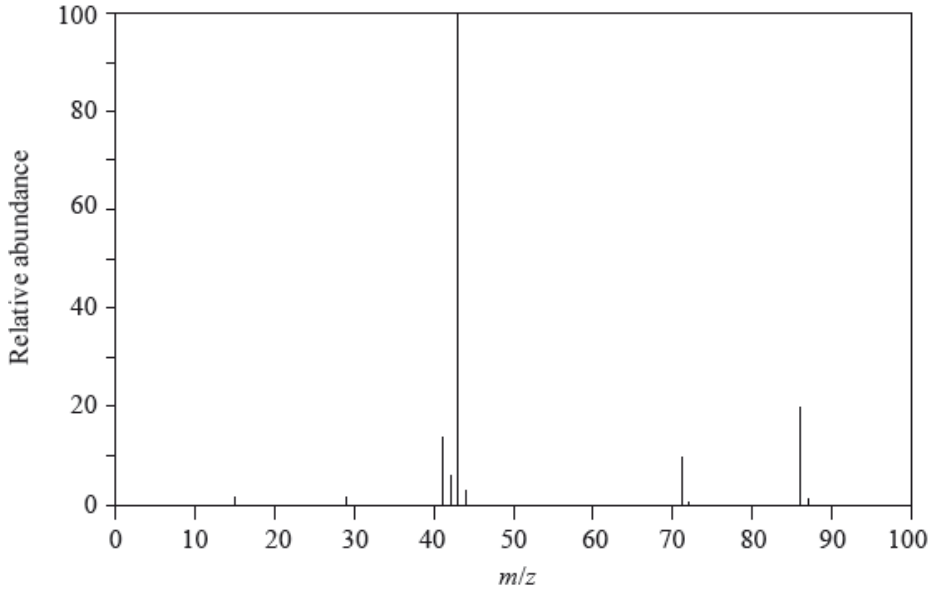
b. (i) bromine. [2]

(ii) hydrogen bromide.

c. When but-1-ene reacts with hydrogen bromide, two possible organic products could be formed but in practice only one organic product is obtained in high yield. Explain the mechanism for this reaction using curly arrows to represent the movement of electron pairs and explain clearly why only one organic product is formed. [4]

Compound **P** contains a carbonyl group (C=O) and has the molecular formula C_3H_6O.

Pentan-2-one has the following mass spectrum.



a. Draw the **two** possible structures of compound **P**. [1]

b. Explain why the infrared spectra of the structures in (a) are very similar. [1]

c. Explain how the mass spectra of the structures in (a) can be used to distinguish between them. [2]

d.i. Deduce the formulas of the species with the *m/z* values at 86, 71 and 43. [3]

$m/z = 86$:

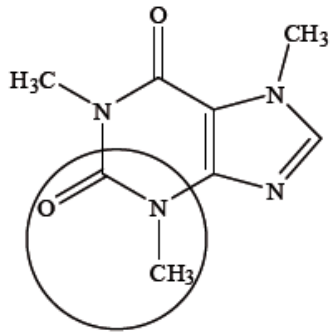
$m/z = 71$:

$m/z = 43$:

d.ii. Suggest a reason for the peak at *m/z* = 43 having an exceptionally high relative abundance. [1]

Caffeine and nicotine are two common stimulants.

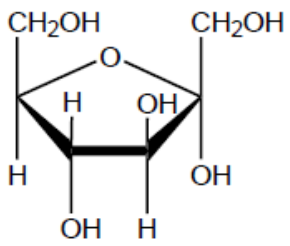
State the name of the functional group circled on the structure of caffeine.



Consider the following lipid and carbohydrate.

$CH_3(CH_2)_4(CH{=}CHCH_2)_2(CH_2)_6COOH$

Linoleic acid, M_r = 280.50



Fructose, M_r = 180.18

In order to determine the number of carbon-carbon double bonds in a molecule of linoleic acid, 1.24 g of the lipid were dissolved in 10.0 cm^3 of non-polar solvent.

The solution was titrated with a 0.300 mol dm^{-3} solution of iodine, I_2.

a.i. Determine the empirical formula of linoleic acid. [1]

a.ii. The empirical formula of fructose is CH_2O. Suggest why linoleic acid releases more energy per gram than fructose. [1]

b.i. State the type of reaction occurring during the titration. [1]

b.ii. Calculate the volume of iodine solution used to reach the end-point. [3]

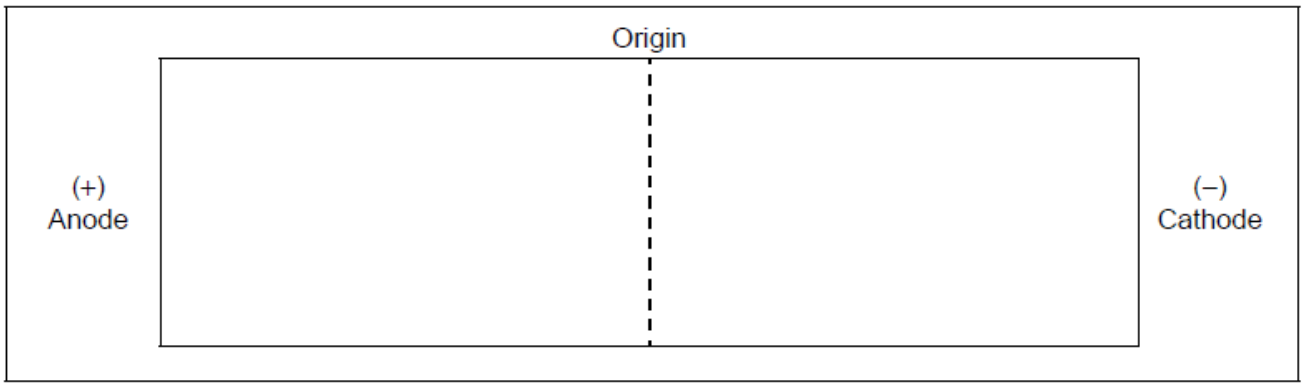
c. Outline the importance of linoleic acid for human health. [2]

Amino acids are usually identified by their common names. Use section 33 of the data booklet.

a. State the IUPAC name for leucine. [1]

b. A mixture of amino acids is separated by gel electrophoresis at pH 6.0. The amino acids are then stained with ninhydrin. [3]

(i) On the diagram below draw the relative positions of the following amino acids at the end of the process: Val, Asp, Lys and Thr.



(ii) Suggest why glycine and isoleucine separate slightly at pH 6.5.

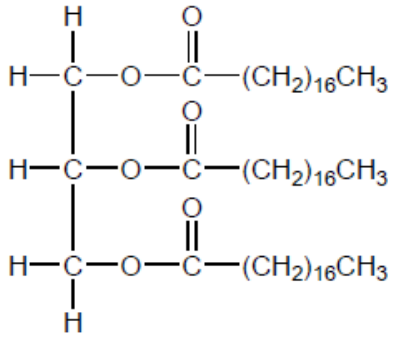
c. Determine the number of different tripeptides that can be made from twenty different amino acids. [1]

d. The fibrous protein keratin has a secondary structure with a helical arrangement. [2]

(i) State the type of interaction responsible for holding the protein in this arrangement.

(ii) Identify the functional groups responsible for these interactions.

Vegetable oils, such as that shown, require conversion to biodiesel for use in current internal combustion engines.



a. State **two** reagents required to convert vegetable oil to biodiesel. [2]

b. Deduce the formula of the biodiesel formed when the vegetable oil shown is reacted with the reagents in (a). [1]

c. Explain, in terms of the molecular structure, the critical difference in properties that makes biodiesel a more suitable liquid fuel than vegetable oil. [2]

d. Determine the specific energy, in $kJ\,g^{-1}$, and energy density, in $kJ\,cm^{-3}$, of a particular biodiesel using the following data and section 1 of the data booklet. [2]

Density = $0.850\ g\,cm^{-3}$; Molar mass = $299\ g\,mol^{-1}$;

Enthalpy of combustion = $12.0\ MJ\,mol^{-1}$.

Specific energy:

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Energy density:

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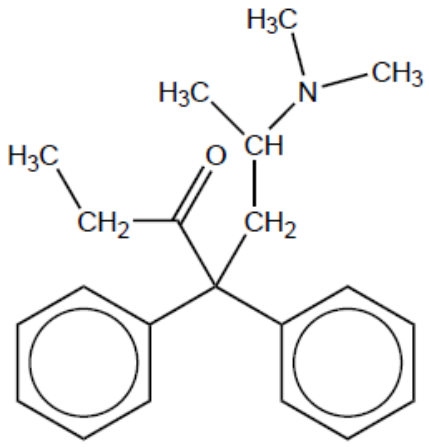
Methadone, a synthetic opioid, binds to opioid receptors in the brain.



Methadone

a. Compare and contrast the functional groups present in methadone and diamorphine (heroin), giving their names. Use section 37 of the data booklet. [2]

One similarity:

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One difference:

. . . . . .

. . . . . .

b. Methadone is sometimes used to help reduce withdrawal symptoms in the treatment of heroin addiction. Outline **one** withdrawal symptom that an addict may experience. [1]

Dehydroepiandrosterone (DHEA) is a substance banned under the World Anti-Doping Code.

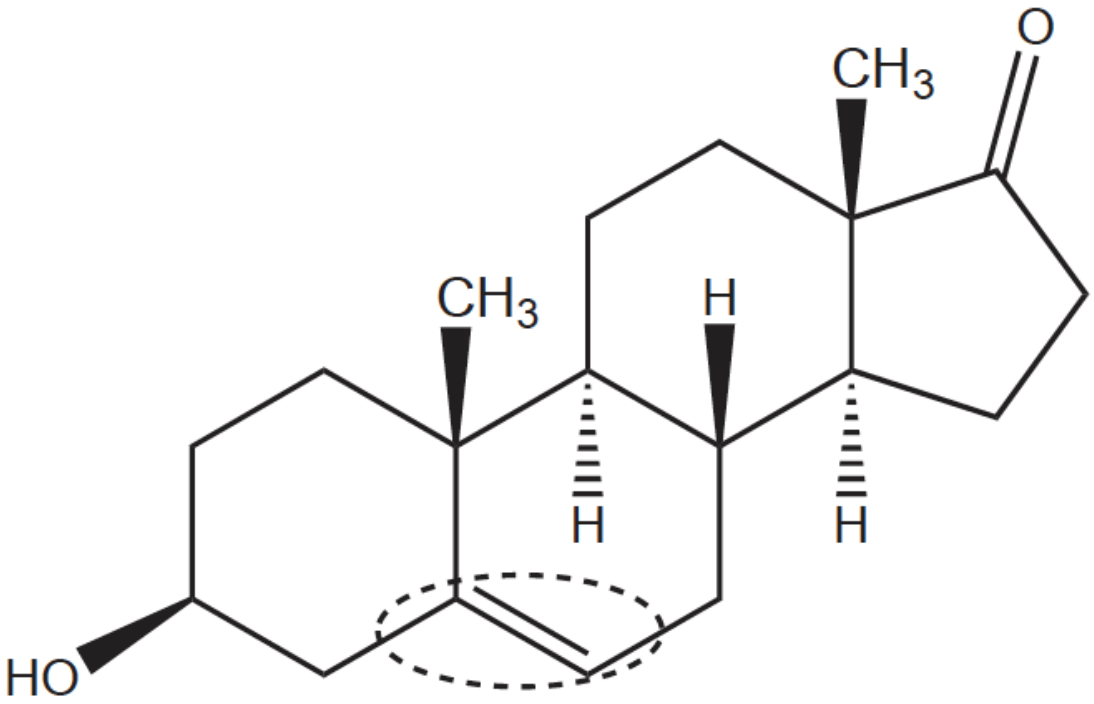
a. Steroid abuse has certain health hazards, some general, some specific to males and some specific to females. Identify **one** health hazard in **each** category. [3]

General Hazard:

Male Hazard:

Female Hazard:

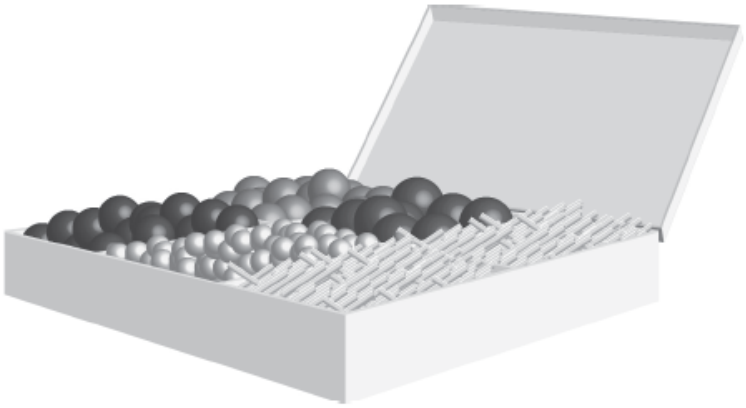
b. (i) State the name of the functional group circled in the DHEA molecule shown below. [2]



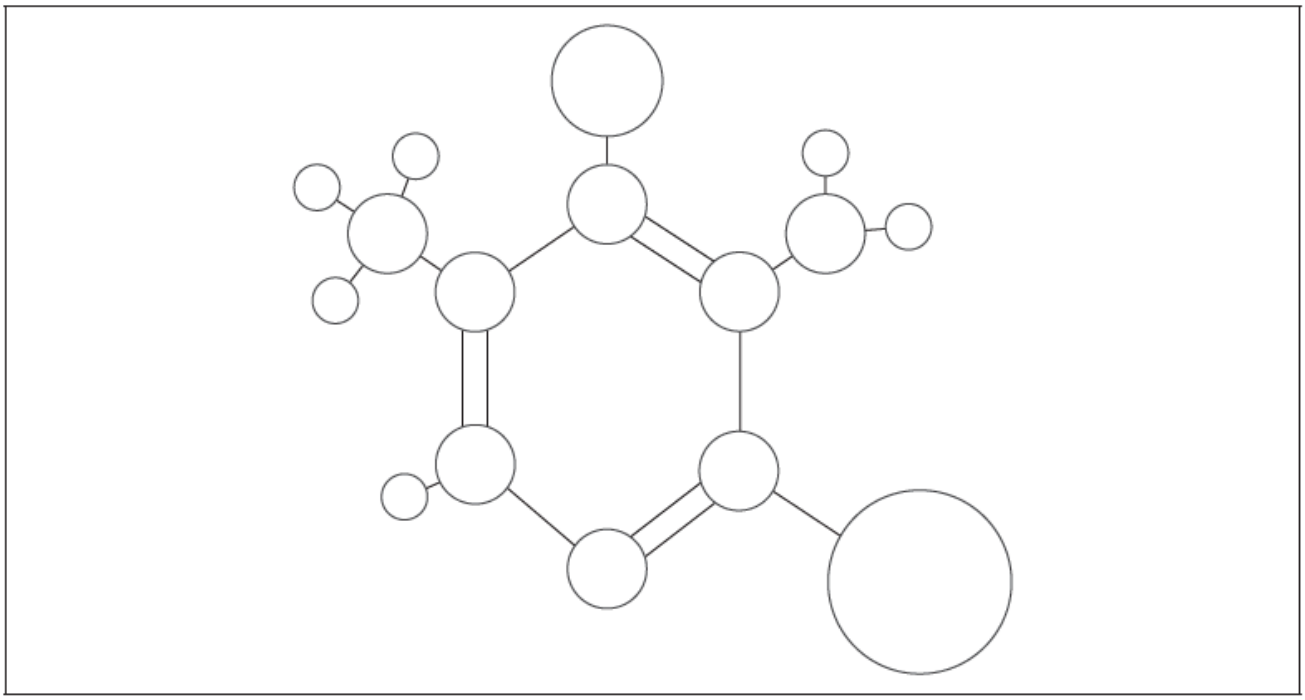
(ii) Identify the characteristic of this structure that classifies it as a steroid.

c. The production of banned steroids has ethical implications. Suggest a reason why steroid research might be supported. [1]

Organic molecules can be visualized using three-dimensional models built from kits such as that pictured below.



[Source: © International Baccalaureate Organization 2018]



[Source: © International Baccalaureate Organization 2018]

a. Describe **two** differences, other than the number of atoms, between the models of ethane and ethene constructed from the kit shown. [2]

b.i. The above ball and stick model is a substituted pyridine molecule (made of carbon, hydrogen, nitrogen, bromine and chlorine atoms). All atoms are shown and represented according to their relative atomic size. [3]

Label each ball in the diagram, excluding hydrogens, as a carbon, C, nitrogen, N, bromine, Br, or chlorine, Cl.

b.ii. Suggest **one** advantage of using a computer generated molecular model compared to a ball and stick 3-D model. [1]

b.iii. Pyridine, like benzene, is an aromatic compound. [1]

Outline what is meant by an aromatic compound.

In a class experiment, students were asked to determine the value of **x** in the formula of a hydrated salt, $BaCl_2 \cdot \mathbf{x}H_2O$. They followed these instructions:

1. Measure the mass of an empty crucible and lid.
2. Add approximately 2 g sample of hydrated barium chloride to the crucible and record the mass.
3. Heat the crucible using a Bunsen burner for five minutes, holding the lid at an angle so gas can escape.
4. After cooling, reweigh the crucible, lid and contents.
5. Repeat steps 3 and 4.

Their results in three trials were as follows:

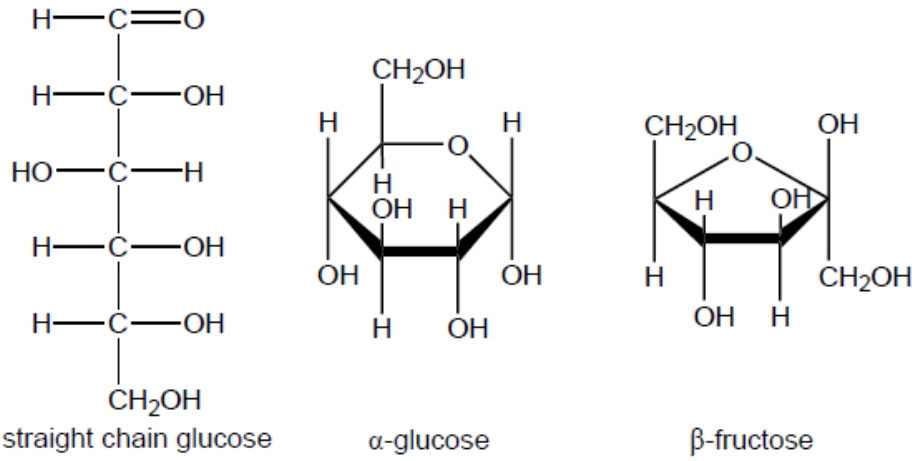
	Trial 1	Trial 2	Trial 3
Mass of crucible + lid / g ±0.001	20.088	20.122	20.105
Mass of crucible + lid + $BaCl_2 \cdot \mathbf{x}H_2O$ before heating / g ±0.001	22.166	22.184	22.186
Mass of crucible + lid + $BaCl_2$ after 1st heating / g ±0.001	21.859	22.080	21.926
Mass of crucible + lid + $BaCl_2$ after 2nd heating / g ±0.001	21.859	21.865	21.927

a. State and explain the further work students need to carry out in trial 2 before they can process the results alongside trial 1. [2]

b. In trial 3, the students noticed that after heating, the crucible had turned black on the outside. Suggest what may have caused this, and how this might affect the calculated value for **x** in the hydrated salt. [2]

c. List **two** assumptions made in this experiment. [2]

Monosaccharides can combine to form disaccharides and polysaccharides.



a. Identify the functional groups which are present in only one structure of glucose. [2]

Only in straight chain form:

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Only in ring structure:

. . . . . .

b. Sucrose is a disaccharide formed from α-glucose and β-fructose. [1]

Deduce the structural formula of sucrose.

c. Starch is a constituent of many plastics. Suggest **one** reason for including starch in plastics. [1]

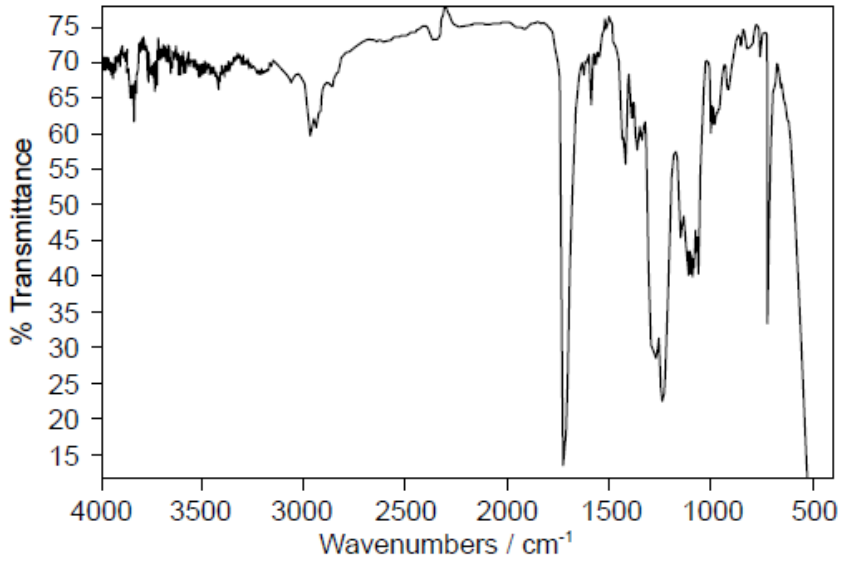
d. Suggest **one** of the challenges scientists face when scaling up the synthesis of a new compound. [1]

Infrared (IR) spectroscopy is often used for the identification of polymers, such as PETE, for recycling.

LDPE and high density polyethene (HDPE) have very similar IR spectra even though they have rather different structures and physical properties.

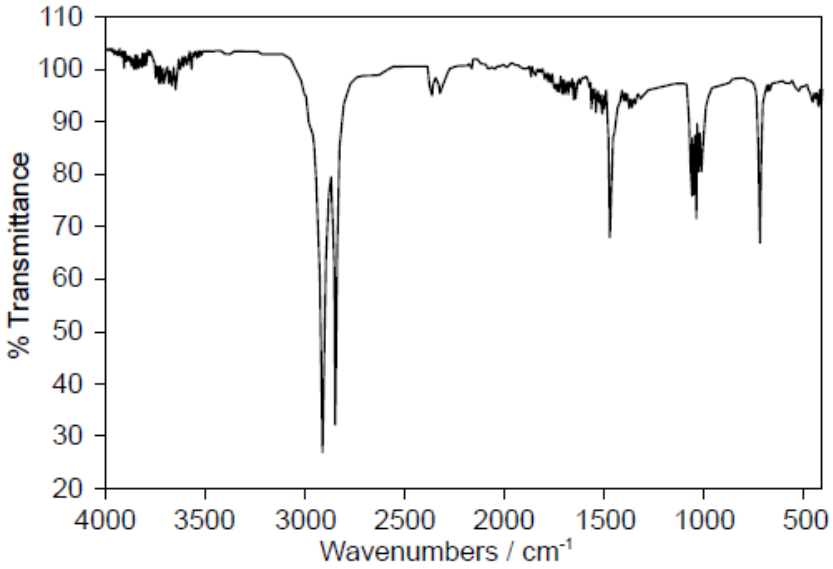
a. Below are the IR spectra of two plastics (**A** and **B**); one is PETE, the other is low density polyethene (LDPE). [3]

A



[Source: www.intechopen.com]

B



[Source: www.andersonmaterials.com]

Deduce, giving your reasons, the identity and resin identification code (RIC) of **A** and **B** using sections 26 and 30 of the data booklet.

A RIC:

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B RIC:

. . . . . .

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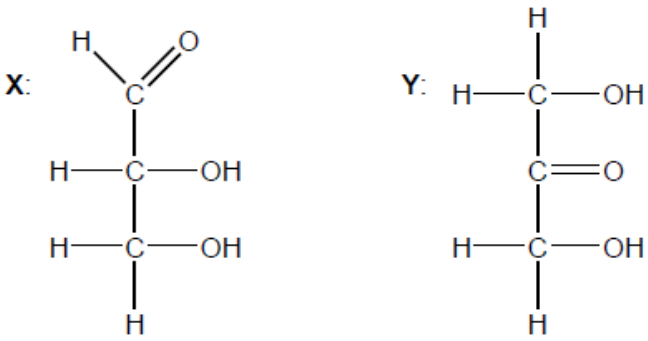
b.i. Describe the difference in their structures. [1]

b.ii. Explain why the difference in their structures affects their melting points. [2]

Carbohydrates are energy-rich molecules which can be synthesized in some plant cells from inorganic compounds.

a. State the raw materials and source of energy used in the process described above. [1]

b. The structures of two molecules, **X** and **Y**, are shown below. [2]



(i) Justify why both these molecules are carbohydrates.

(ii) Distinguish between these molecules in terms of their functional groups.

c. Amylose is an unbranched polysaccharide composed of repeating units of glucose. [3]

(i) Draw the structure of the repeating unit of amylose. Use section 34 of the data booklet.

(ii) Amylose is a major component of starch. Corn starch can be used to make replacements for plastics derived from oil, especially for packaging. Discuss **one** potential advantage and **one** disadvantage of this use of starch.

Advantage:

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Disadvantage:

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