H432/02 Synthesis & analytical techniques June 2017

Model Answers

Level	A Level
Subject	Chemistry A
Exam Board	OCR
Paper Code	H432/02
Paper	Synthesis & analytical techniques
Booklet	Model Answers

Time allowed: **135 minutes**

Score: **/100**

Percentage: **/100**

Grade Boundaries:

A*	A	B	C	D	E
>85%	73%	60%	47%	34%	21%

Question 1

A chemist compares the rates of hydrolysis of 1-chloropropane and 1-bromopropane in ethanol.

Which reagent in aqueous solution should be used?

A. Silver chloride

[✓ B. Silver nitrate]

C. Potassium chloride

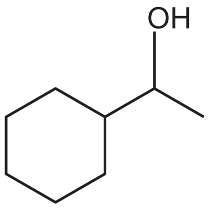
D. Potassium nitrate

[1]

- Ag^+ ions react with halide ions to form the **halogen precipitates** $AgCl$ and $AgBr$ in aqueous solution.
- Silver nitrate is a soluble salt which releases Ag^+ ions in aqueous solution and is regularly used to test for halogens.
- A is incorrect as silver chloride is **insoluble** hence does not release silver ions.
- C and D are incorrect as these compounds do not contain silver.

Question 2

How can the molecule below be described?



A. Aromatic and alicyclic

B. Aliphatic and unsaturated

C. Aromatic and unsaturated

[✓ D. Alicyclic and saturated]

[1]

- Alicyclic compounds contain a **cyclic** part and an **aliphatic** part as the molecule shown does have.
- It is also **saturated** as there are no **carbon carbon double** bonds present.
- A and C are incorrect as it is not aromatic as there is no **benzene** ring present.
- B is incorrect as it is **saturated**.

Complete combustion of an organic compound forms 40 cm^3 of carbon dioxide and 40 cm^3 of water vapour, under the same conditions of temperature and pressure.

Which molecular formula could the organic compound have? **[1]**

A C_3H_8

B. C_2H_2O

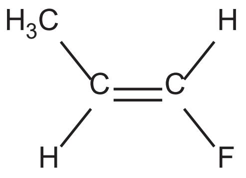
[✓ C. C_2H_4O]

D. C_2H_3N

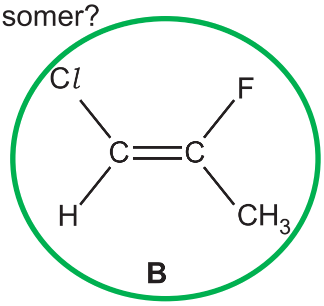
- Since the same conditions of temperature and pressure then the ratio of moles to volume is proportional.
- The questions states that there are 40cm^3 of CO_2 and 40cm^3 of H_2O, therefore the ratio of C : H in the products is 1 : 2.
- This ratio of C : H must be present in the reactants due to the law of conservation of mass, and is only present in opcíon C.
- A, B and D are thus incorrect.

Question 4

Which molecule is a *Z*-isomer?



A



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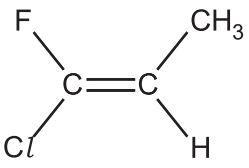
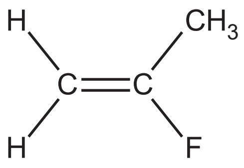


C



D

[1]

- In the Cahn-Ingold-Prelog system groups are assigned priority based on their atomic number, with the groups of **higher atomic number** having higher priority.
- If the higher priority groups or atoms are on the **same side** of the double bond then the compound is a *Z* isomer.
- This only occurs in B since C*l* and F are both high priority groups.
- A and C are incorrect as these are E isomers since the groups are on **opposite** sides of the double bond.
- D is incorrect as there are two hydrogens on the left carbon so *E*/*Z* isomerism cannot occur.

Which type of reaction has the greatest atom economy?

A Substitution

B Hydrolysis

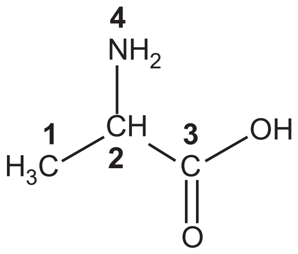
C Elimination

[✓ **D** Addition]

[1]

- The equation for atom economy is:
    - ○ Atom economy = $\frac{total\ M_r\ of\ the\ desired\ product}{total\ M_r of\ all\ reactants}$ x 100
- The highest economy occurs in addition reactions where molecules are being brought together to form compounds, hence **all products are considered desired** so the economy is 100 %.
- A, B and C are incorrect as all of these reactions produce side products which lower the percentage economy.

Four atoms, **1–4**, are labelled in the structure below.



Which atom has a trigonal planar arrangement of bonds around it? **[1]**

A. Atom 1

B. Atom 2

[✓ C. Atom 3]

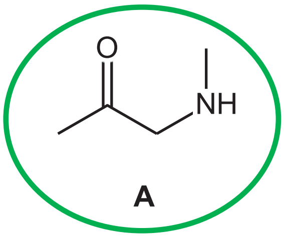
D. Atom 4

- Carbon 3 forms a **trigonal planar** arrangement as it has **3 bonding pairs** and no lone pairs.
- Carbons 1 and 2 both adopt a **tetrahedral** arrangement.
- Group 4 is incorrect as the nitrogen has a lone pair of electrons hence it will form a **pyramidal** shape.
- Hence A, B and D are incorrect.

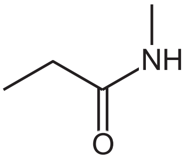
Question 7

Which molecule is a secondary amine?

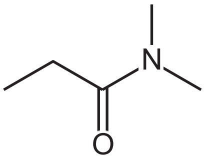
[1]



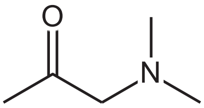
A



B

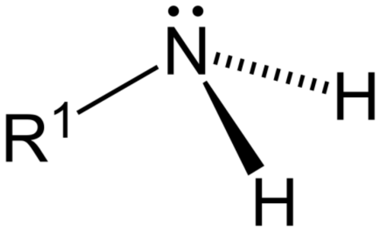
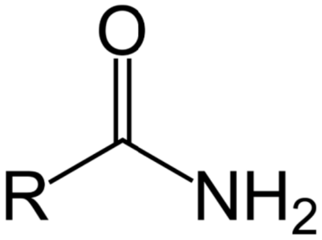


C



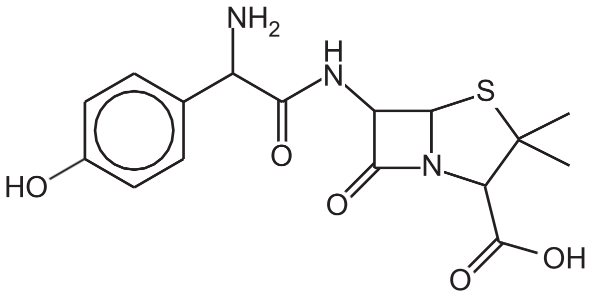
D

- A is correct as there is an amine group present which is attached to two carbons, hence it is a **secondary** amine.
- Options B and C are incorrect as both of these are **amides** and not amines.
- D is incorrect as there are three carbons attached to the nitrogen atom, hence it is a **tertiary** amine.

	
Primary amine	Primary amide

Question 8

What is the number of chiral centres in the molecule below? **[1]**



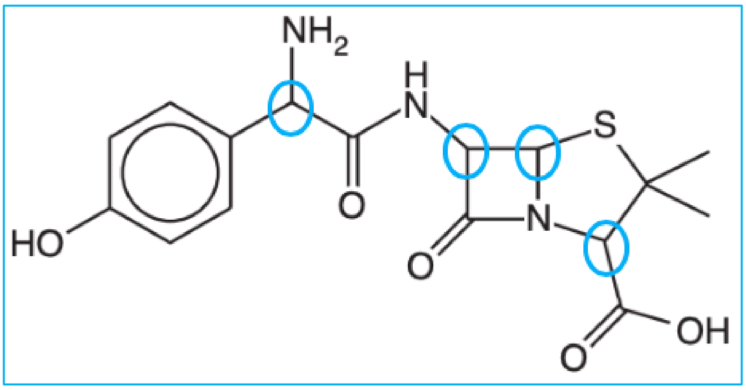
A. 2

B. 3

[✓ C. 4]

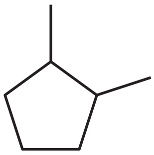
D. 5

- A chiral centre is a carbon atom bonded to four different groups.
- Starting on the left-hand side identify the groups attached to each carbon atom and identify those carbon atoms that are chiral.
- There are 4 chiral carbons which are identified on the diagram of the molecule below.
- A, B and D are thus incorrect.



Question 9

What is the molecular formula of the compound below?



A C_7H_{10}

B C_7H_{12}

[✓ **C** C_7H_{14}]

D C_7H_{16}

[1]

- Start on the bottom left hand side, pick the first carbon atom and start counting in clockwise direction all of the carbon atoms. Do the ring first and then the side arms.
- Then count the hydrogens, starting from the same point and in the same order.
- The ring has 5 carbons and 2 carbon on the side chains, 14 hydrogens in total so C_7H_{14}.
- A, B and D are thus incorrect.

Question 10

Equal amounts of the four compounds are added to the same volume of water.

Which compound would produce the most acidic solution?

A. CH_3CONH_2

B. CH_3COOH

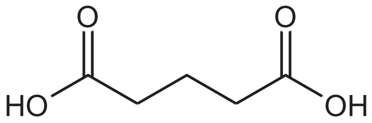
C. CH_3COOCH_3

[✓ D. CH_3COCl]

[1]

- Compound D is an **acyl chloride**. These compounds hydrolyse in water to produce HCl which is a strong acid.
- A is incorrect as amides are very weakly **basic**.
- B is incorrect as carboxylic acids are only **mildly acidic**.
- C is incorrect as esters are **non-acidic**.

The compound below is analysed by ^{1}H NMR spectroscopy.



How many peaks are observed in the ^{1}H NMR spectrum?

A. 5

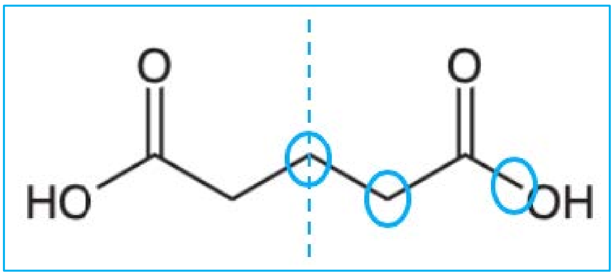
B. 4

[✓ C. 3]

D. 2

[1]

- The compound contains a plane of symmetry in the middle as shown by the dashed line on the diagram below.
- There are **three** different proton environments around the plane as shown by the circles in the diagram.
- A, B and D are thus incorrect.



Question 12

0.1 mol of $HOOCCH_2COOH$ are reacted with 0.1 mol of aqueous NaOH.

How many molecules of water are formed?

[✓ **A** 6.02×10^{22}]

B 3.01×10^{22}

C 6.02×10^{23}

D 3.01×10^{23}

[1]

- The acid used is **di-protic** as it dissociates to produce **2 protons** per molecule. The base used only produces 1 hydroxyl group per molecule, so in effect the base is the **limiting** reagent.
- Therefore the amount of water molecules produced is Avogadro's constant multiplied by the concentration of the base used:
  - $(0.1) \times (6.02 \times 10^{23}) = 6.02 \times 10^{22}$.
- B, C and D are therefore incorrect.

Question 13

Which reagents could be used to prepare $CH_3CH_2CONHCH_3$?

[✓ A. $CH_3CH_2COCl + CH_3NH_2$]

B. $CH_3CH_2CONH_2 + CH_3Br$

C. $CH_3CH_2COONa + CH_3NH_2$

D. $CH_3CH_2COCH_3 + NH_3$

[1]

- **Acyl chlorides** react with **amines** to produce the product molecule which is an **amide**.
- The amine acts as the nucleophile through lone pair donation from the nitrogen atom to the electron deficient species.
- B, C and D are incorrect as none of these reactions produce amides.

Question 14

Ethane reacts with chlorine by radical substitution to form chloroethane.

Which radical(s) is/are present in the mechanism?

1 $H\bullet$

2 $Cl\bullet$

3 $C_2H_5\bullet$

A. 1, 2 and 3

B. Only 1 and 2

[✓ C. Only 2 and 3]

D. Only 1

[1]

- Radical substitution reactions occur in three stages: initiation, propagation and termination. The overall mechanism is shown below:
    - $Cl_2 \longrightarrow \mathbf{2Cl\bullet}$ Initiation Stage
    - $C_2H_6 + Cl\bullet \longrightarrow \mathbf{C_2H_5\bullet} + HCl$ Propagation Stage
    - $C_2H_5\bullet + Cl_2 \longrightarrow C_2H_5Cl + Cl\bullet$
    - $2Cl\bullet \longrightarrow Cl_2$ Termination Stage
    - $C_2H_5\bullet + C_2H_5\bullet \longrightarrow C_4H_{10}$
- Hydrogen radicals do not appear in the mechanism, hence A, B and D are incorrect.

Question 15

Which compound(s) is a/are structural isomer(s) of $C_6H_{12}O_2$?

1 hexanoic acid

2 ethyl butanoate

3 propyl propanoate

[✓ A. 1, 2 and 3]

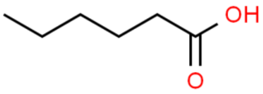
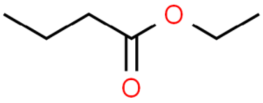
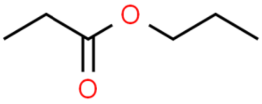
B. Only 1 and 2

C. Only 2 and 3

D. Only 1

[1]

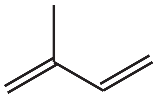
- Structural isomers are compounds that have the same molecular formula but different structural formula as the bonding arrangement between the atoms is different.
- All three compounds are structural isomers with the molecular formula of $C_6H_{12}O_2$ as shown below.
- B, C and D are thus incorrect.

Displayed formula			
Name	Hexanoic acid	Ethyl butanoate	Propyl propanoate
Molecular Formula	$C_6H_{12}O_2$	$C_6H_{12}O_2$	$C_6H_{12}O_2$

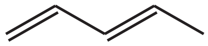
Question 16

This question is about unsaturated hydrocarbons.

(a) Compound **A** and compound **B** are isomers.



compound A



compound B

Compound **A** has a lower melting point than compound **B**.

Suggest why. **[2]**

Compound **A** is branched so it has less points of contact or surface interaction between molecules. The induced dipole–dipole interactions or London dispersion forces are weaker and so less energy is required to break them.

Branching prevents molecules from getting as close together as the molecules in straight chains. This causes a decrease in the **surface area** and hence the intermolecular forces are less so the boiling point **decreases** with increased branching.

(b) Compound **C**, $CH_3CH_2CH=CHCH_2CH_2OH$, exists as *cis* and *trans* stereoisomers.

(i) Name compound **C**. **[1]**

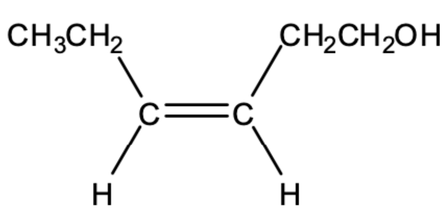
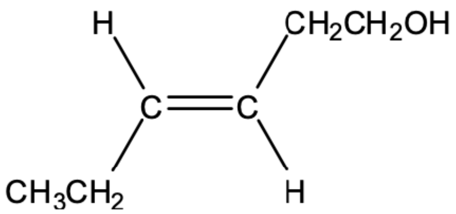
Hex-3-en-1-ol

There are 6 carbons so the name begins with hex-, hydroxyl group on the end so -ol, and carbon carbon double bond on carbon number 3 counting from the right, so hex-3-en-1-ol.

(ii) Define the term *stereoisomers*. **[1]**

Stereoisomers are molecules with the same structural formula **AND** different arrangement of atoms **in space OR** different **spatial** arrangement of atoms.

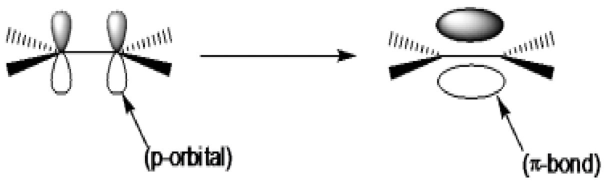
(iii) Draw the structures of the *cis* and *trans* stereoisomers of compound **C**. **[2]**

	
Cis (H atoms on the same side)	*Trans* (H atoms on opposite sides)

(c) The C=C group in an alkene contains a π-bond.

Complete the diagram below to show how p-orbitals are involved in the formation of a π-bond.

[1]



Two p-orbitals shown as a "dumb-bell" added to structure on left and labelled.

AND

π-bond on structure on right formed from the overlap of the p-orbitals. It's good practice to shade either the top or bottom sections of both dumbbells, so that you're showing where each π bond comes from.

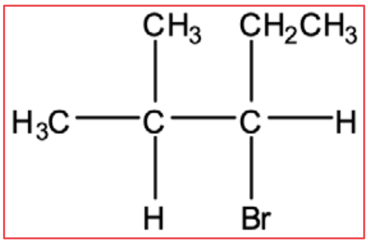
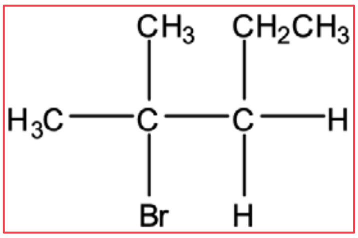
(d) Compound **D**, shown below, reacts with hydrogen bromide by electrophilic addition. A mixture of two organic compounds, **E** and **F**, is formed.

compound D

(i) Suggest how an HBr molecule can act as an electrophile. **[1]**

Electrophiles are electron pair acceptors. The H atom of HBr accepts a pair of electrons which causes the carbon carbon double bond to break, allowing for addition to occur at the carbocation.

(ii) Draw the structures of the two organic compounds **E** and **F**. **[2]**

 $H_3C-\overset{CH_3}{\underset{H}{C}}-\overset{CH_2CH_3}{\underset{Br}{C}}-H$	 $H_3C-\overset{CH_3}{\underset{Br}{C}}-\overset{CH_2CH_3}{\underset{H}{C}}-H$
E	**F**

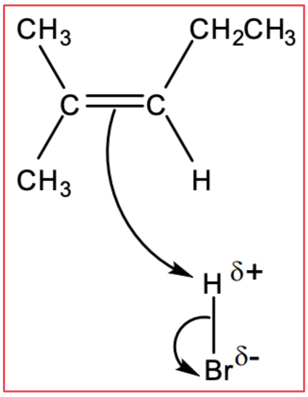
(iii) Outline the mechanism of the reaction between compound **D** and hydrogen bromide to form **either** compound **E or** compound **F**.

Include curly arrows and relevant dipoles.

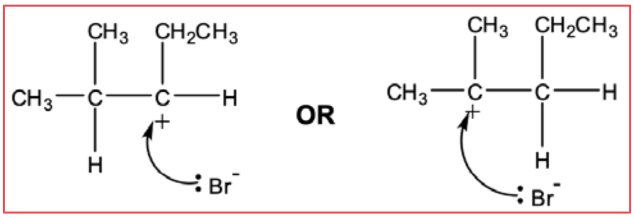
[3]

Diagram must show a curly arrow from the middle of the C=C bond to the H of H–Br.

Correct dipole shown on H–Br with a δ+ on the H and a δ- on the Br **AND** a curly arrow showing the breaking of the H–Br bond, starting in the middle and ending on the Br atom.



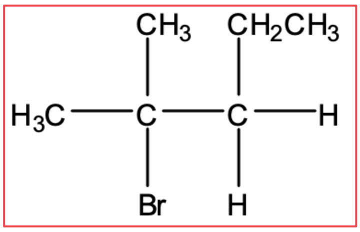
The diagram must show the correct carbocation with a full positive charge **AND** curly arrow from the electron pair on the Br^- to the C^+ of the carbocation.



(iv) Which of **E** or **F** is the major organic product?

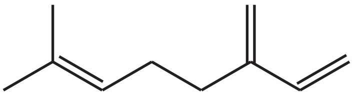
Explain your answer.

[1]



The major product formed is 2-bromo-2-methylpentane. The **carbocation** intermediate in the formation of 2-bromo-2-methylpentane is a secondary tertiary carbocation and is thus more stable than the carbocation in the formation of the other product which is a secondary carbocation.

(e) Myrcene, $C_{10}H_{16}$, is a naturally occurring hydrocarbon containing more than one carbon-carbon double bond.



myrcene

(i) Reaction of 204 mg of myrcene with hydrogen gas produces a saturated alkane.

Calculate the volume of hydrogen gas, in cm^3 and measured at RTP, needed for this reaction.

Show your working.

[2]

Step	**Working out**
1. For each carbon carbon double bond, work out how many hydrogens are needed.	One hydrogen molecule is needed per double bond. There are three double bonds so 3 moles of H_2 are needed per mole of myrcene.
2. Calculate the moles of myrcene.	*n*(myrcene) = $\frac{204 \times 10^{-3}}{136.0}$ = 1.5(0) x 10^{-3} (mol)
3. Multiply by three as per step 1 to find the moles of hydrogen needed.	*n*(hydrogen) = 3 x 1.5(0) x 10^{-3} = 4.5 x 10^{-3}
4. Convert to volume using the molar volume of gas.	Volume of H_2 = 4.5 x 10^{-3} x 24000 = 108 cm^3

(ii) β-Carotene is a naturally occurring unsaturated hydrocarbon found in carrots. A β-carotene molecule contains 40 carbon atoms, has two rings, and a branched chain.

0.0200 mol of β-carotene reacts with 5.28 dm^3 of hydrogen gas to form a saturated hydrocarbon.

Using molecular formulae, construct a balanced equation for this reaction.

Include relevant calculations and reasoning.

[4]

Step	**Working out**
1. Calculate the moles of hydrogen.	nH$_2$) = $\frac{5.28}{24}$= 0.22(0) (mol)
2. Divide the result from step one by the number of moles of β-carotene to find the ratio of β-carotene : hydrogen molecules.	Double bonds = $\frac{0.220}{0.0200}$ = 11 So the ratio is 1 : 11 for β-carotene : hydrogen molecules.
3. Multiply by three as per step 1 to find the moles of hydrogen needed.	n(hydrogen) = 3 x 1.5(0) x 10^{-3} = 4.5 x 10^{-3}
4. Convert to volume.	Volume of H_2 = 4.5 x 10^{-3} x 24000 = 108 cm^3
5. Work out the formula of the saturated product.	The rings each contain 4 carbons and there are two rings. The general formula is thus the same as an alkane but minus 2 for the rings, so C_nH_{2n-2}. The H's are therefore (2 x 40)-2 = 78. The formula of β-carotene is thus $C_{40}H_{78}$.
6. Use the information to work out the balanced equation.	So far we have: $C_{40}H\_\_ + 11H_2 \longrightarrow C_{40}H_{78}$ Therefore 56 H's are required on the LHS to balance the equation, which is thus: $C_{40}H_{56} + 11H_2 \longrightarrow C_{40}H_{78}$

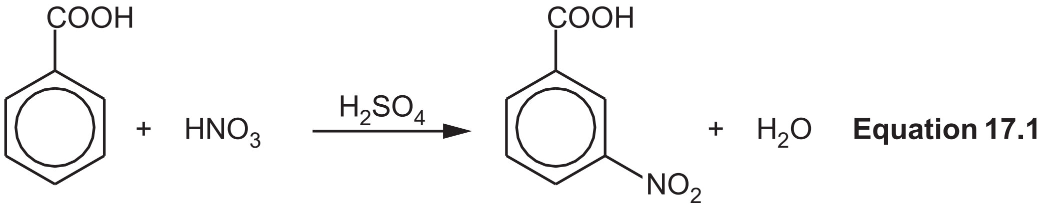
(Total 20 marks)

Question 17

This question is about the chemistry of aromatic compounds.

(a) Benzoic acid can be nitrated by concentrated nitric acid in the presence of concentrated sulfuric acid as a catalyst, as shown in **Equation 17.1**.

The organic product of this reaction is 3-nitrobenzoic acid.



benzoic acid **3-nitrobenzoic acid**

(i) Outline the mechanism for this nitration of benzoic acid.

Show how H_2SO_4 behaves as a catalyst. **[5]**

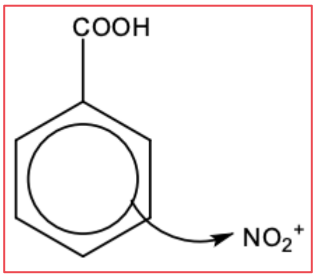
Generation of electrophile

$HNO_3 + H_2SO_4 \longrightarrow H_2O + HSO_4^- + NO_2^+$

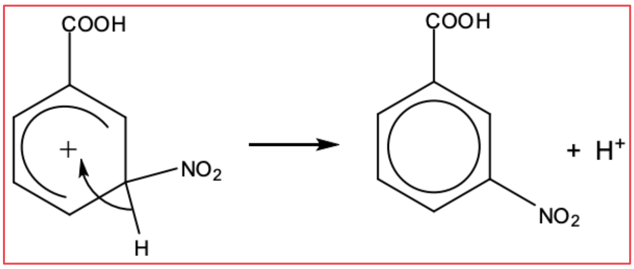
Sulfuric acid catalyses the reaction by dehydrating the HNO_3 to produce the NO_2^+ ion.

Electrophilic substitution

The diagram must show the curly arrow from π-bond to NO_2^+, making sure that it is clear the arrow starts at the π-bond.



The curly arrow must come back from the middle of the C-H bond to reform π-ring **AND** H^+ as product. The nitro group must be substituted on the **third carbon atom** as stated in the question. The **broken circle** therefore must be drawn with the opening facing carbon number 3.



Regeneration of catalyst

$H^+ + HSO_4^- \longrightarrow H_2SO_4$

(ii)* A chemist carries out the reaction in **Equation 17.1** using 4.97 g of benzoic acid.

The chemist obtains 3-nitrobenzoic acid as an impure solid.

The chemist purifies the solid to obtain 4.85 g of 3-nitrobenzoic acid.

Describe a method to obtain a pure sample of 3-nitrobenzoic acid from the impure solid, determine the percentage yield and check its purity.

[6]

1. Purification

- Recrystallisation
- Dissolve impure solid in minimum volume of hot water/solvent. Using the minimum amount avoids product remaining in solution after cooling.
- Cool solution and filter solid
- Wash with cold water/solvent and dry

2. Percentage yield

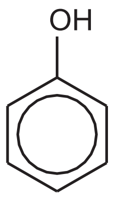
Using the equation percentage yield = $\frac{actual\ yield}{theoretical\ yield}$ x 100:

- n(benzoic acid) used = $\frac{4.97}{122}$ = 0.0407 (mol)
- n(3-nitrobenzoic acid) made = $\frac{4.85}{167}$ = 0.0290 (mol)
- Percentage yield = $\frac{0.0290}{0.0407}$ x 100 = 71.3 (%)

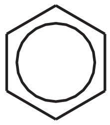
3. Checking purity

- Obtain melting point
- Compare to known values
- Pure sample will have a sharp melting point very close to data book value whereas a range indicates that the sample is not pure.

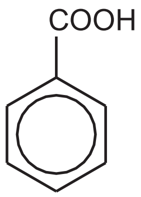
(b) A student investigates the relative ease of nitration of phenol, benzene, and benzoic acid.



phenol



benzene



benzoic acid

The student finds that the conditions required for the nitration of each compound are different, as shown in **Table 17.1**.

Compound	**phenol**	**benzene**	**benzoic acid**
Conditions required for nitration	Dilute HNO_3 20 °C No catalyst	Concentrated HNO_3 55 °C H_2SO_4 catalyst	Concentrated HNO_3 100 °C H_2SO_4 catalyst

Table 17.1

(i) State the trend in the relative ease of nitration of phenol, benzene, and benzoic acid. **[1]**

Analysing the data in the table, phenol is the most easily nitrated/ most reactive as it requires only 20°C and no catalyst is used. Benzene and benzoic acid both need a catalyst but benzoic acid requires a temperature of 100°C compared to 55°C for benzene. So benzoic acid is the least easily nitrated /least reactive. Therefore the order of ease of nitration, starting with the easiest is phenol ⟶ benzene ⟶ benzoic acid.

(ii) Apply your knowledge of the bonding in arenes to explain the trend in part **(b)(i)**. **[3]**

Reactivity of phenol

There is a lone pair of electrons on the oxygen atom which is **partially delocalised** into the ring system. This increases the electron density making the ring **more susceptible** to electrophilic attack.

Reactivity of benzoic acid

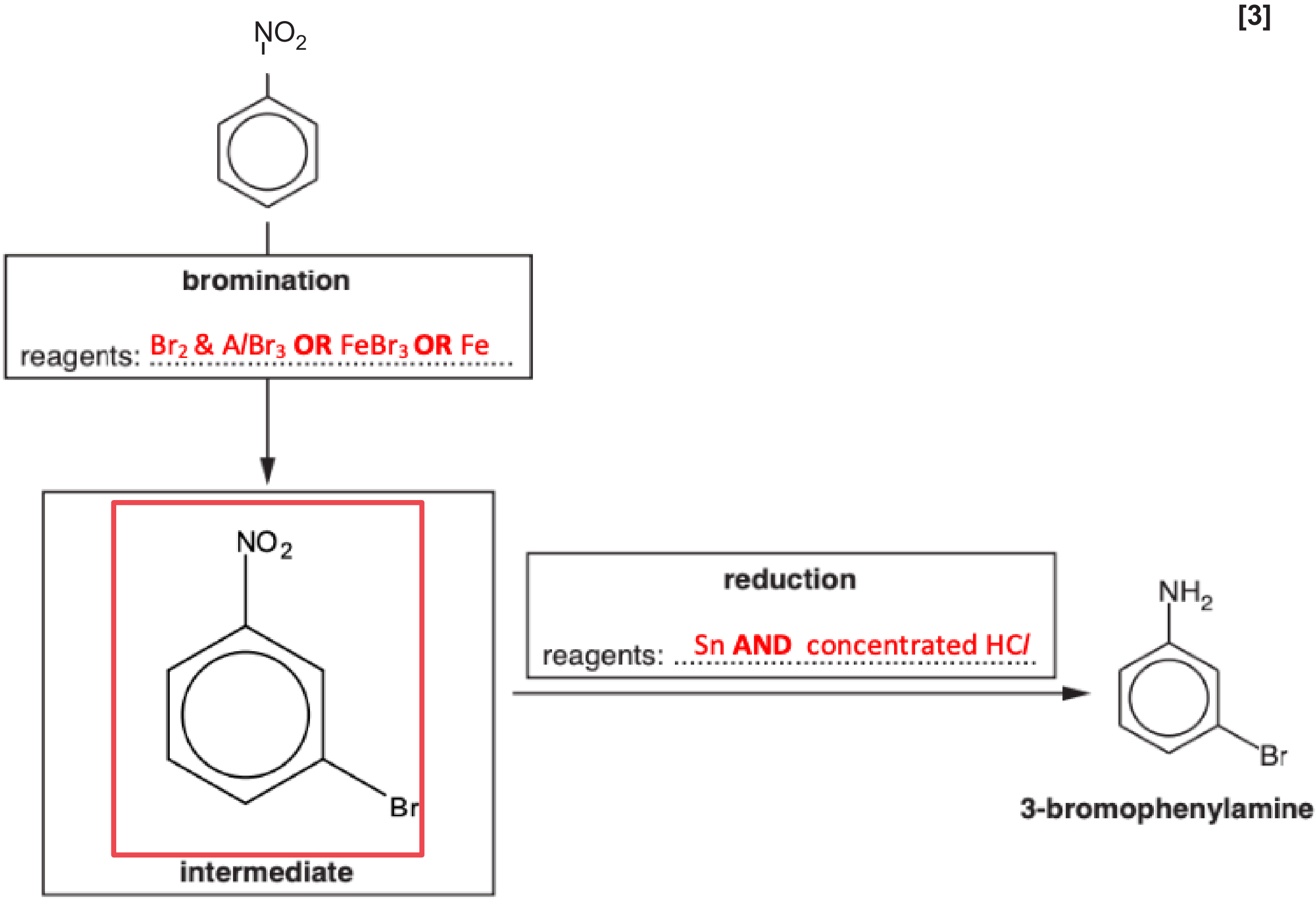
The –COOH group on benzoic acid is an electron withdrawing group as the carbon atom is bonded to an oxygen atom which is **electronegative**. In terms of resonance structures this can produce a slight positive charge on the carbon atom that thus attracts electrons from the ring.

This decreases the electron density making the ring **less susceptible** to electrophilic attack.

(c) A student synthesises 3-bromophenylamine, shown below, starting from nitrobenzene.

(i) Complete the flowchart showing the structure of the intermediate and the **formulae** of the reagents for each stage.

[3]

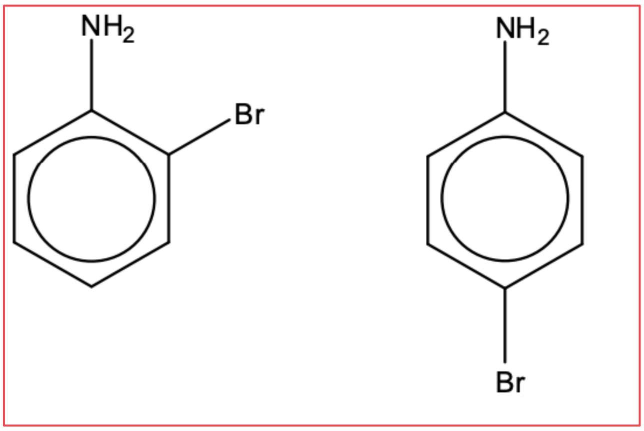


(ii) Another student attempts the same synthesis but carries out reduction **before** bromination. The student was surprised to find that two structural isomers of 3-bromophenylamine had been formed instead of the desired organic product.

Explain this result and suggest the structures of the two isomers that formed.

[3]

NH_2 is 2,4 directing as nitrogen, similar to the phenol group, has a **lone pair of** electrons which can delocalise into the ring system making NH_2 2,4,6 directing. 2 and 6 are the same molecule, hence NH_2 is 2 and 4 directing, producing **ortho isomers** as shown in the diagrams below.



(Total 21 marks)

This question is about organic compounds containing nitrogen.

(a) Sodium cyanide, NaCN, can be reacted with many organic compounds to increase the length of a carbon chain.

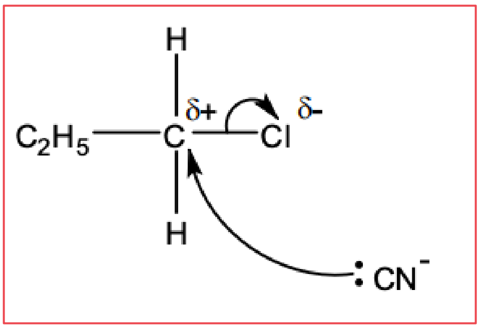
(i) 1-Chloropropane, $CH_3CH_2CH_2Cl$, reacts with ethanolic sodium cyanide by nucleophilic substitution.

Outline the mechanism for this reaction.

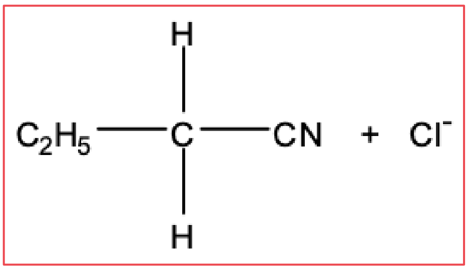
Include curly arrows, relevant dipoles and the structure of the organic product.

[3]

The diagram must show a curly arrow from the lone pair of electrons on the ^-CN to the carbon atom of C–C*l* bond. There must be a dipole shown on C–C*l* bond, $C^{\delta+}$ and $Cl^{\delta-}$, **AND a** curly arrow from the C–C*l* bond to the C*l* atom.



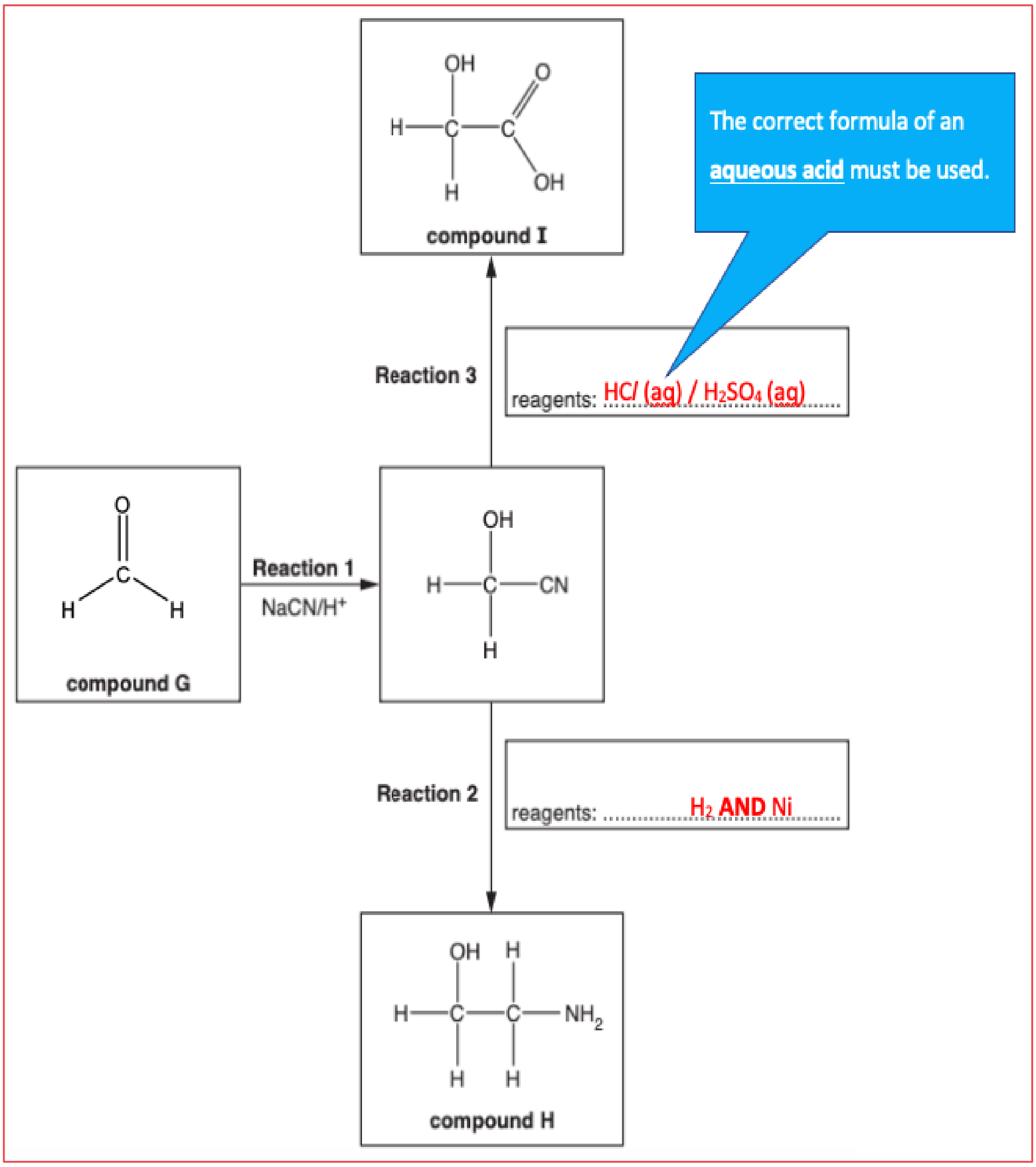
The correct organic product must be shown **AND** the Cl^-.



(ii) Compound **G** is used to synthesise compounds **H** and **I** as shown in the flowchart below.

Complete the flowchart showing the structure of compound **G** and the **formulae** of the reagents for **Reaction 2** and **Reaction 3**.

[3]



The correct formula of an aqueous acid must be used.

reagents: HC*l* (aq) / H_2SO_4 (aq)

reagents: H_2 AND Ni

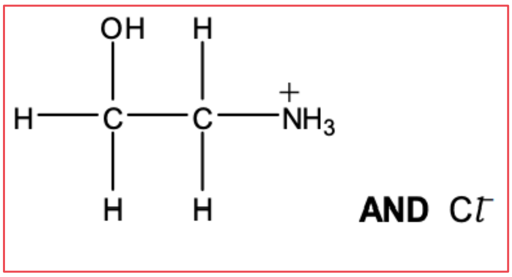
(iii) Compound **H** reacts with dilute hydrochloric acid to form a salt.

Explain why compound **H** can react with dilute hydrochloric acid and suggest a structure for the salt formed.

[2]

This occurs as the nitrogen atom has a **lone pair of electrons** and therefore accepts a proton/H^+.

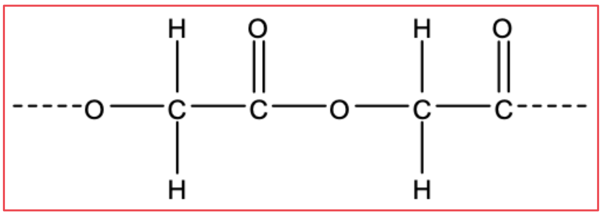
Correct structure of the salt as shown below with the chloride cation included after cleavage from the H atom. The plus charge must be displayed on the nitrogen atom.



(iv) Compound **I** is the monomer for the biodegradable polymer **J**.

Draw **two** repeat units of polymer **J** and suggest a reason why it is biodegradable.

[3]

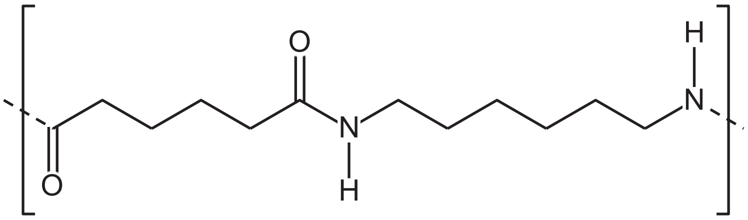


Molecule H contains an alcohol group at one end and a carboxylic group at the other end.

An ester link is formed during condensation polymerisation.

Polymer J is biodegradable because the ester bond in the polyester can be hydrolysed which disrupts the polymer chain and breaks it down.

(b) The repeat unit of Nylon 6,6 is shown below.

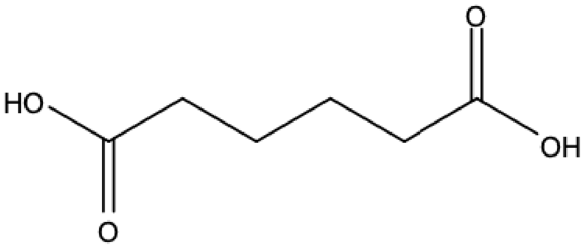
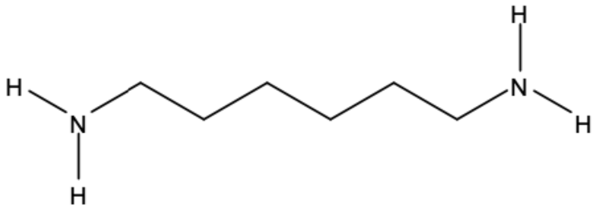


Nylon 6,6

(i) Draw the structures of **two** monomers that can be used to form Nylon 6,6.

[2]

There are two possible monomers. One has -COOH groups on either end and the other has -NH_2 groups on either end as shown below.

	
-COOH Monomer	-NH_2 monomer

(ii) A sample of Nylon 6,6 has a relative molecular mass of 21500.

Estimate the number of repeat units in the sample.

Give your answer as a **whole** number.

[1]

Divide the molecular mass of Nylon 6, 6 by the relative molecular mass of one of the repeat units:

$$n = \frac{21500}{226} = 95.1 = 95.$$

(Total 14 marks)

This question is about alcohols.

(a) Construct an equation for the complete combustion of an unsaturated alcohol with 5 carbon atoms.

[1]

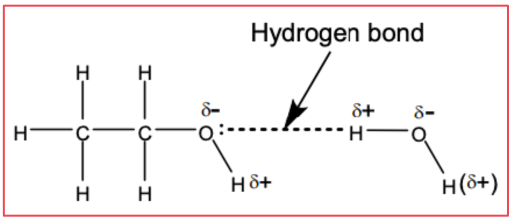
$C_5H_{10}O + 7O_2 \longrightarrow 5CO_2 + 5H_2O$

(b) Many alcohols, including ethanol, are soluble in water.

(i) Explain, with the aid of a diagram, why ethanol is soluble in water.

Include relevant dipoles and lone pairs.

[2]



The diagram must show a water molecule and an ethanol molecule with at least one $H^{\delta+}$ and one $O^{\delta-}$ on BOTH molecules.

Hydrogen bond **between one lone pair** on an O atom in one of the molecules and the H atom of another. **AND** Hydrogen bonding stated or labelled on diagram.

(ii) The solubility of hexan-1-ol and hexane-1,6-diol in water is shown below in **Table 19.1**.

Alcohol	Solubility in water / $g\,dm^{-3}$
hexan-1-ol	5.9
hexane-1,6-diol	500

Table 19.1

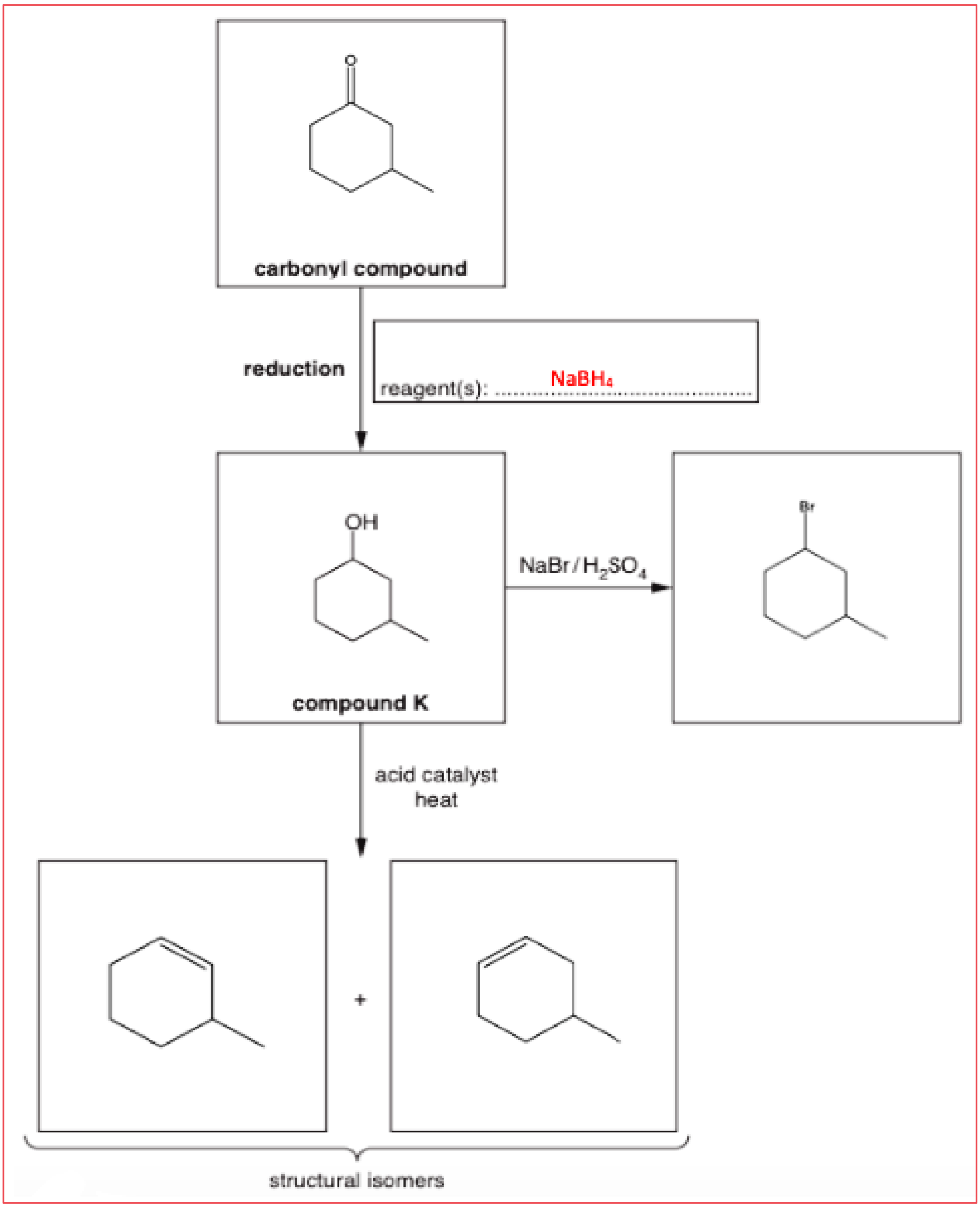
Explain the difference in solubility of hexan-1-ol and hexane-1,6-diol.

[1]

Hexane-1,6-diol has more OH groups than hexan-1-ol so forms more hydrogen bonds with water which makes it more soluble.

(c) Alcohols are important in organic synthesis and can be formed by the reduction of carbonyl compounds.

(i) Complete the flowchart by filling in each box. **[5]**



(ii) What is the name of compound **K**? **[1]**

3-methylcyclohexanol

There is a methyl group on carbon number 3 and an -OH group on carbon number 1.

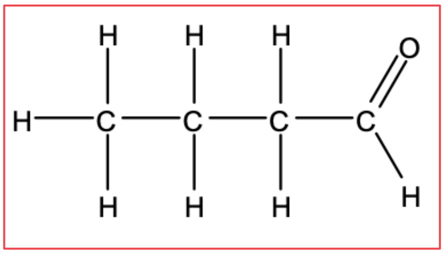
(d) Butan-1-ol can be oxidised to form two different organic products, depending on the reaction conditions used.

Describe both oxidation reactions of butan-1-ol.

For each reaction include

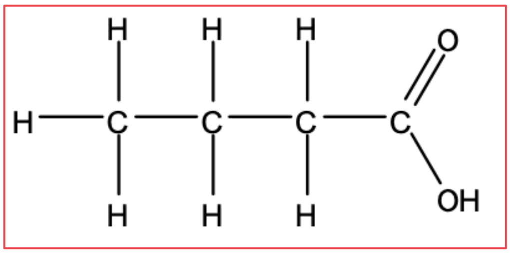
- the structure of the organic product
- a balanced equation
- the essential reaction conditions.

In your equations you may use [O] to represent the oxidising agent. **[5]**



$CH_3CH_2CH_2CH_2OH + [O] \longrightarrow CH_3CH_2CH_2CHO + H_2O$

Butan-1-ol is a primary alcohol which undergoes oxidation in acidic conditions and distillation to produce an aldehyde product, in this case butanal.



$CH_3CH_2CH_2CH_2OH + 2[O] \longrightarrow CH_3CH_2CH_2COOH + H_2O$

If butan-e-ol is refluxed and the product is not removed via distillation, then the reaction continues on and produces a carboxylic acid, in this case butanoic acid. The oxidising agent most commonly used is potassium dichromate (VI) acidified with dilute H_2SO_4.

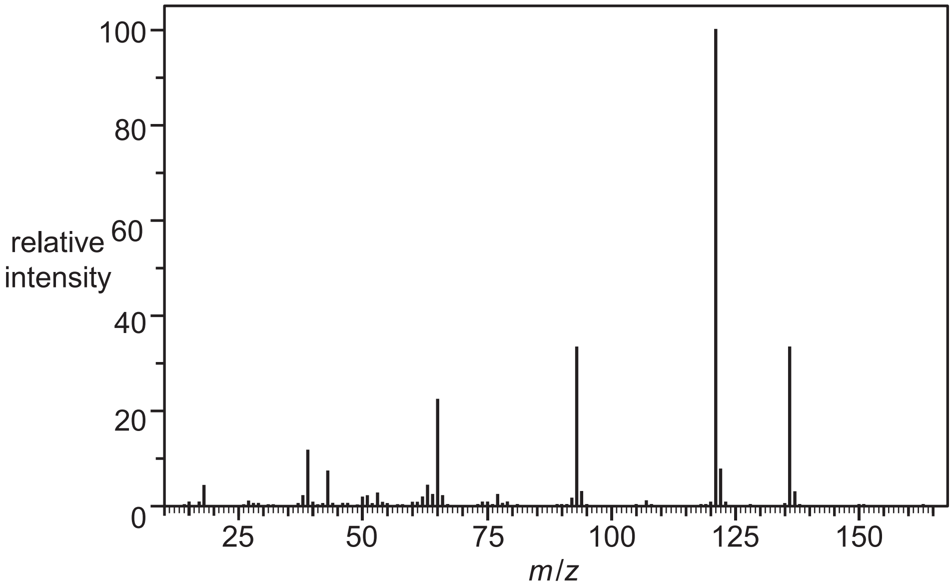
(Total 15 marks)

A chemist analyses a naturally occurring aromatic compound.

(a) The percentage composition and mass spectrum of the compound are shown below.

Percentage composition by mass: C, 70.58%; H, 5.92%; O, 23.50%.

Mass spectrum



Determine the molecular formula of the compound.

Show your working. **[3]**

Step	**Working out**
1. Calculate the **mole ratio** by dividing the percentages by the relative atomic mass of each element.	$C = \frac{70.58}{12.0}$: $H = \frac{5.92}{1.0}$: $O = \frac{23.50}{16.0}$ So 5.88 : 5:92 1.47
2. Divide across by the lowest result to obtain the **empirical formula.**	C_4H_4O
3. Use the *m/z* ratio to determine the molecular formula.	*m/z* = 136 (8 x 12) + (8 x 1) + (2 x 16) = 132.0 so molecular formula is $C_8H_8O_2$.

(b) Qualitative tests are carried out on the aromatic compound. The results are shown below.

Test	**Acidity**	**Na_2CO_3(aq)**	**2,4-DNP**	**Tollens' reagent**
Observation	pH = 5	No observable change	Orange precipitate	No observable change

Determine the functional groups in the compound. Explain your reasoning.

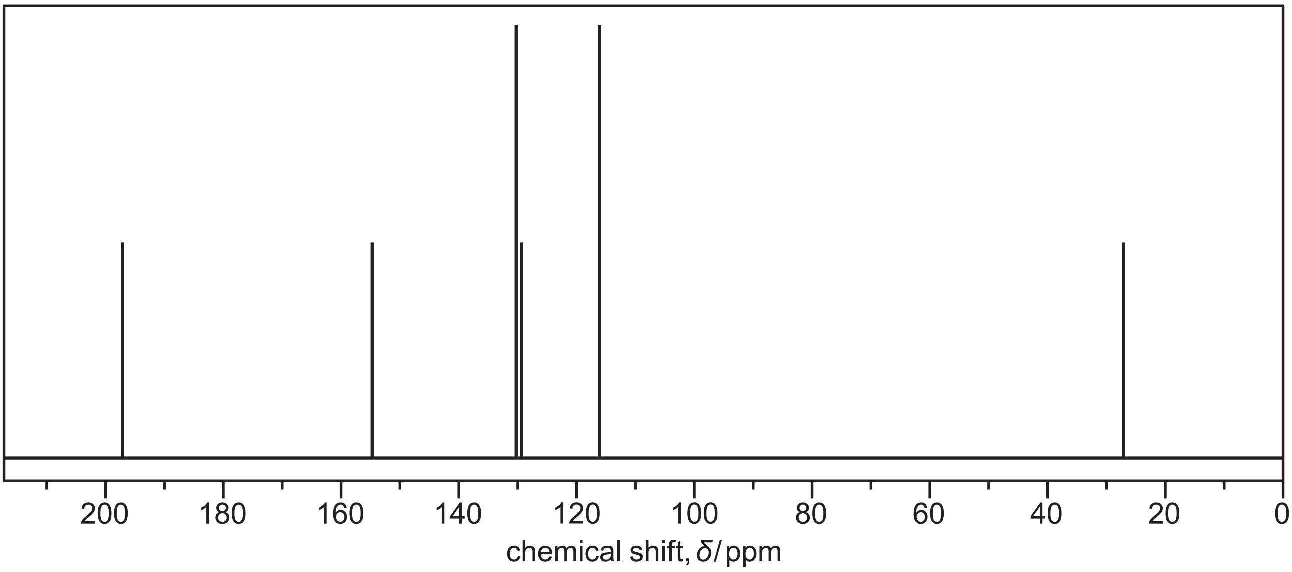
[3]

Phenol are weak acids **AND** there is no reaction with Na_2CO_3 so the compound is most likely not a carboxylic acid.

Reaction with 2,4-DNP(H) or Brady's reagent produces an orange precipitate which is 2,4-dinitrophenylhydrazone formed when the NH_2 group of 2,4-DNP adds across the C=O group, which is followed by the removal of a water molecule.

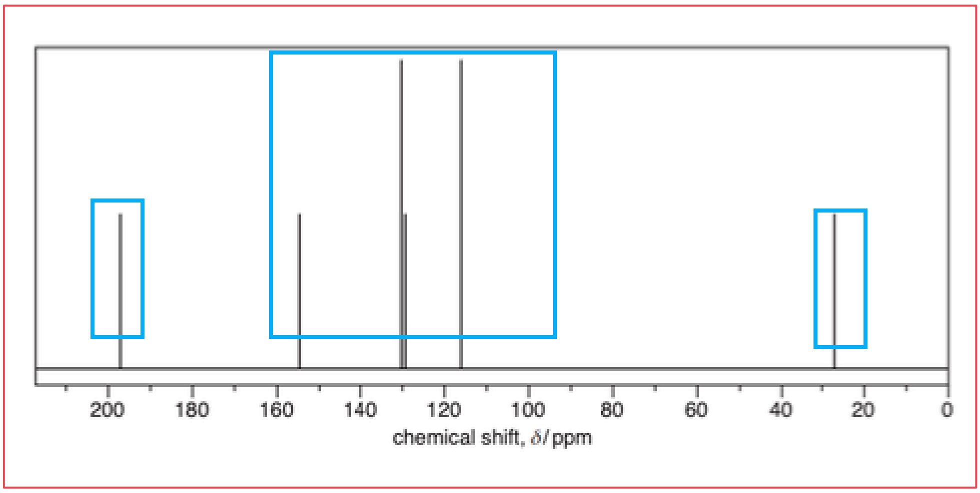
Tollens' reagent test produces no observable change so compound is not an aldehyde, so it must be a ketone.

(c) The carbon-13 NMR spectrum of the compound is shown below.

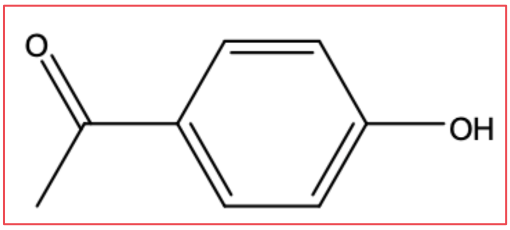


Using the spectrum and the results from **(a)** and **(b)**, determine the structure of the compound. Explain your reasoning.

Carbon NMR analysis



Start by adding the phenol group to one side of the benzene ring. The peaks between 110–160 ppm correspond to the four aromatic carbon environments. The compound contains a C=O between which corresponds to the peak at 190 - 200 ppm **AND** a C-C at 20-30 ppm which corresponds to the methyl group. The C=O must be attached to the benzene ring as it is a ketone and not an aldehyde.

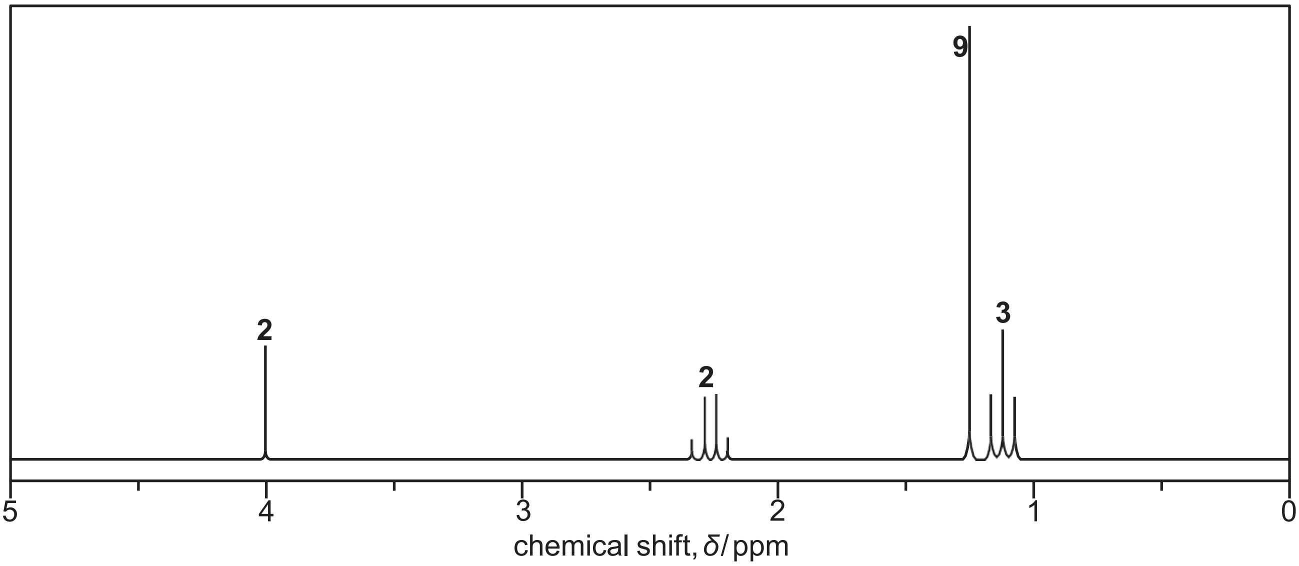


Structure of compound

[3]

(Total 9 marks)

Compound **L** is an organic compound containing carbon, hydrogen and oxygen only.
The ^{1}H NMR spectrum of compound **L** is shown below.
The numbers by the peaks are the relative peak areas.



Compound **L** is refluxed with aqueous hydrochloric acid, forming two organic compounds **M** and **N**. The infrared spectra of **M** and **N** are shown below.

Infrared spectrum of M

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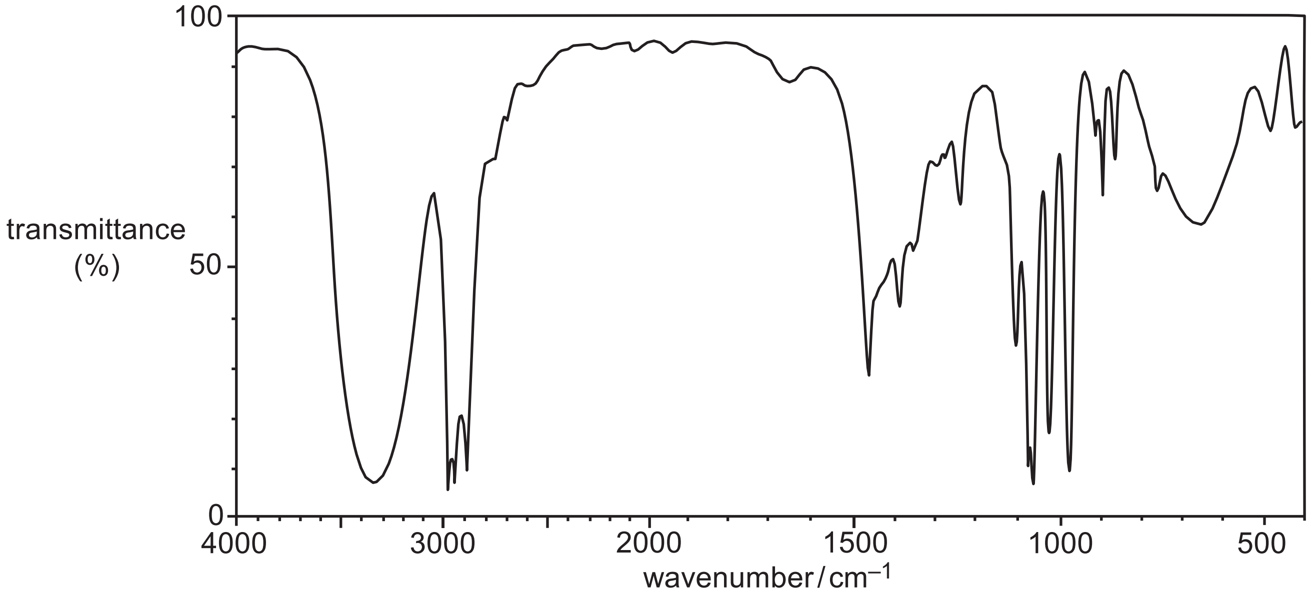
Infrared spectrum of N



Use the information provided to suggest a structure for compound **L**.

Show **all** of your reasoning.

[6]

No Answer available

(Total 6 marks)