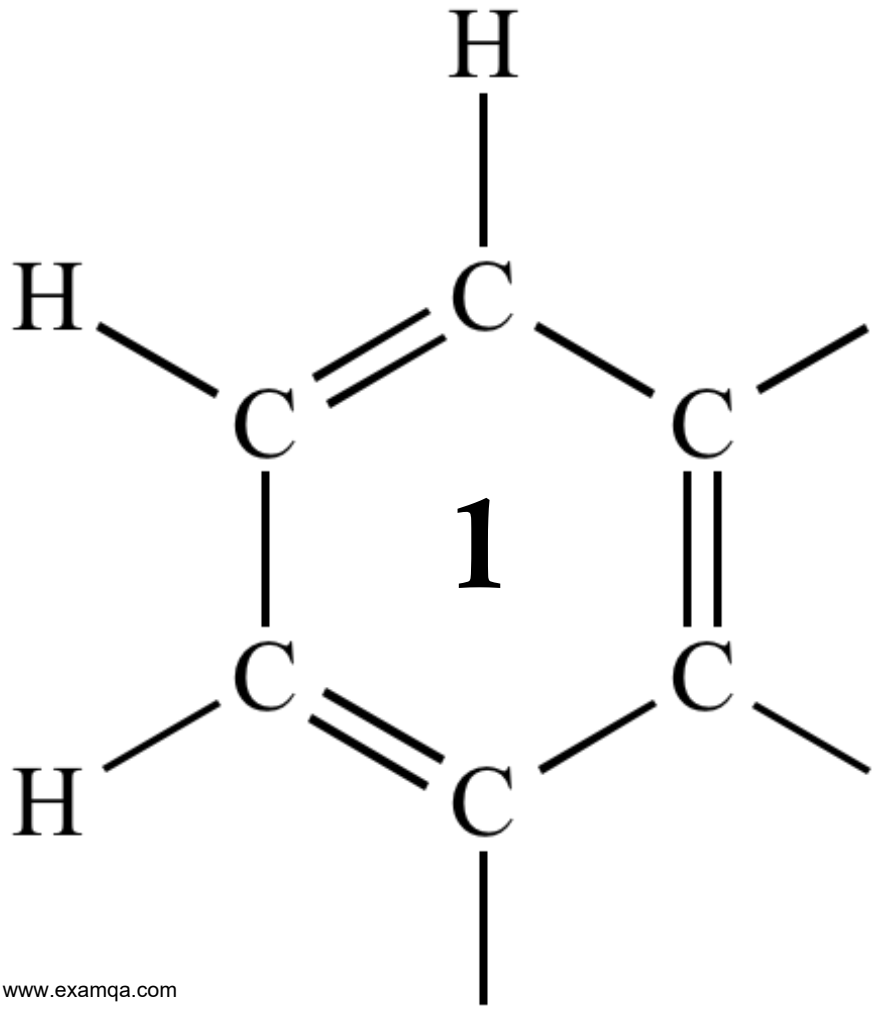
LONDON SCIENCE COLLEGE

OCR A2 CHEMISTRY

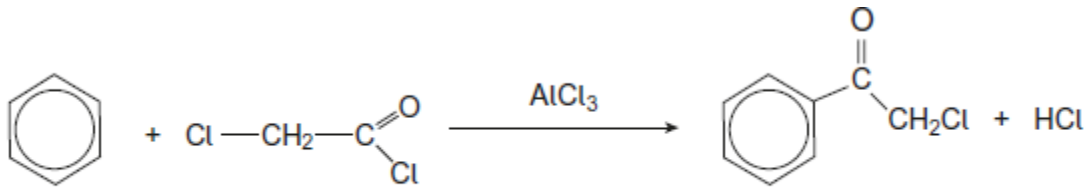
MODULE 6.4

ANALYSIS



1 Compound **X** ($ClCH_2COCl$) is used as a reagent in organic synthesis.

(a) One important reaction of **X** is in the preparation of compound **P** as shown.



X **P**

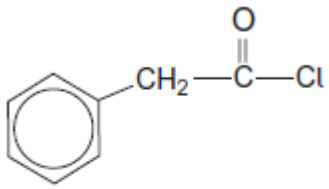
(i) Draw the structure of the electrophile formed by the reaction of **X** with $AlCl_3$.

(1)

(ii) Outline the mechanism for the reaction of the electrophile from part **(a)(i)** with benzene in the preparation of **P**.

(3)

(b) Compound **Q** is an alternative product that could be formed when **X** reacts with benzene.



Q

Describe how you could distinguish between **P** and **Q** by a test-tube reaction.
Give the reagent used and the observation with each compound.

Reagent .....

Observation with **P** .....

Observation with **Q** .....

(3)

(c) **X** is also used to make the compound $HOCH_2COOH$. This compound is polymerised to form the polymer known as PGA. PGA is used in surgical sutures (stitches).

(i) Draw the repeating unit of PGA.

(1)

(ii) Production of PGA occurs via a cyclic compound. Two $HOCH_2COOH$ molecules react together to form the cyclic compound and two molecules of water.

Draw the structure of this cyclic compound.

(1)

(d) Poly(propene) is also used in surgical sutures.

(i) Draw the repeating unit of poly(propene).

(1)

(ii) Suggest an advantage of surgical sutures made from PGA rather than from poly(propene).
Explain your answer.

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(2)
(Total 12 marks)

2 Compound **R** contains 61.0% carbon and 11.9% hydrogen by mass. The remainder is oxygen. The mass spectrum of **R** contains a molecular ion peak at *m*/*z* = 118.

(a) Use these data to show that the molecular formula of **R** is $C_6H_{14}O_2$.

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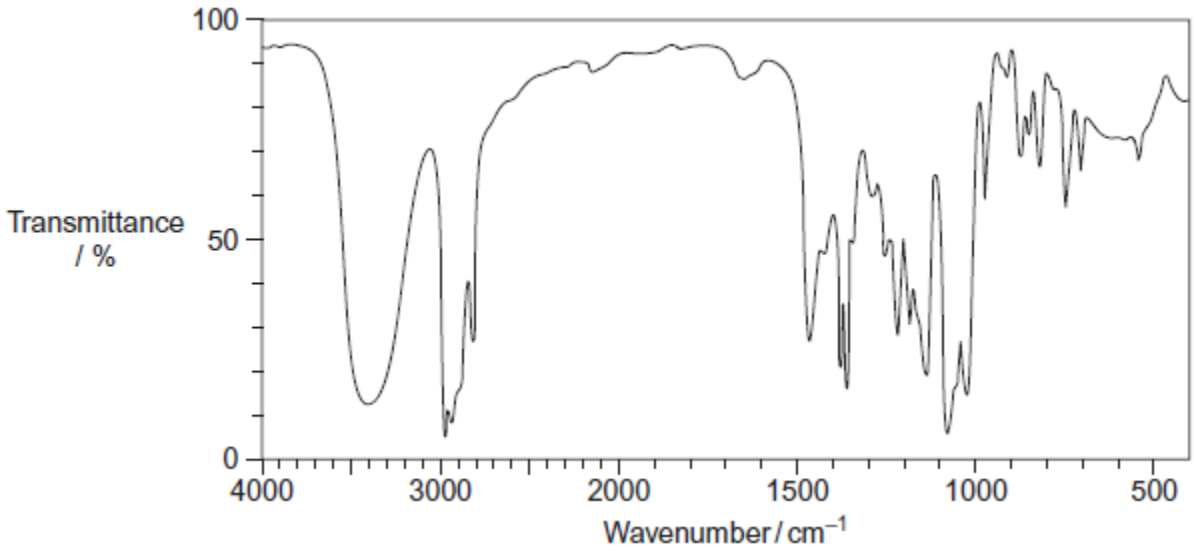
(3)

(b) The infrared spectrum of **R** ($C_6H_{14}O_2$) is shown below.



The proton n.m.r. spectrum of **R** contains five peaks. The chemical shift values, integration ratios and splitting patterns of these peaks are given in the table.

Chemical shift/ppm	3.8	3.2	3.1	1.4	1.1
Integration ratio	2	3	1	2	6
Splitting patterns	triplet	singlet	singlet	triplet	singlet

When **R** is warmed with acidified potassium dichromate(VI) a green solution is formed.

Use **Table A** and **Table B** on the data sheet and all of the data provided in the question to deduce the structure of **R**.

In your answer, explain how you have used the data provided in the question.

(9)

(Total 12 marks)

3 The infrared spectrum (**Figure 1**) and the ^{1}H NMR spectrum (**Figure 2**) of compound **R** with molecular formula $C_6H_{14}O$ are shown.

Figure 1

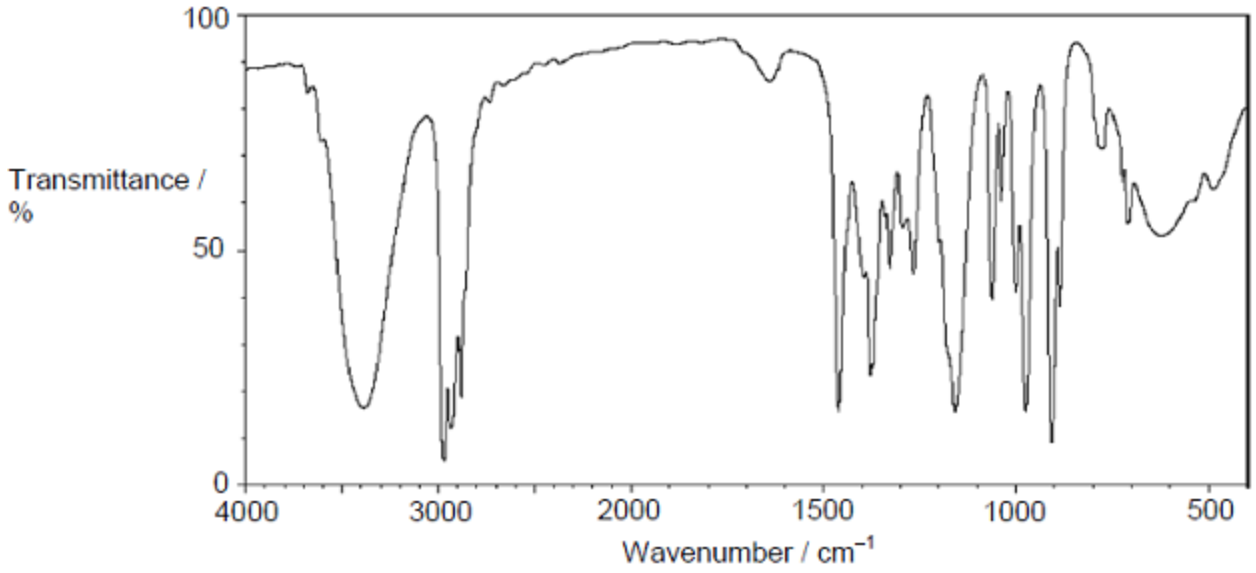
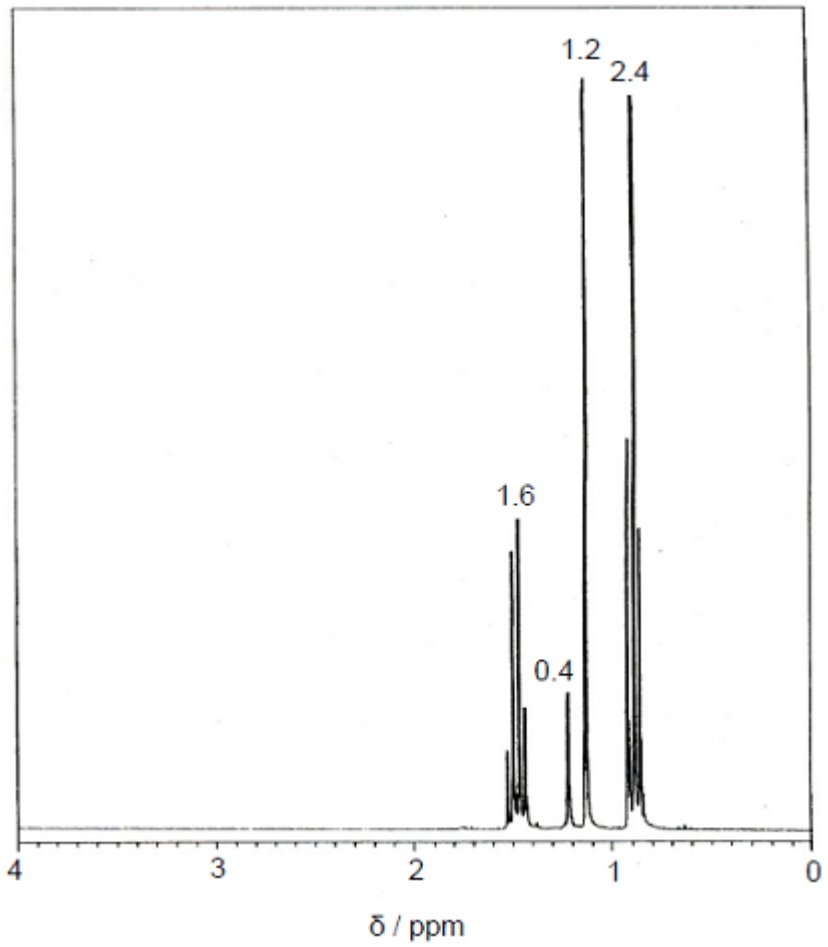


Figure 2



The relative integration values for the NMR peaks are shown on **Figure 2**.

Deduce the structure of compound **R** by analysing **Figure 1** and **Figure 2**.
Explain each stage in your deductions.

Use **Table A** and **Table B** on the Data Sheet.

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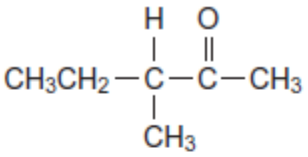
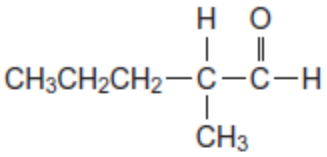
(Total 8 marks)

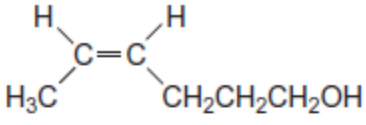
4 The following five isomers, **P**, **Q**, **R**, **S** and **T**, were investigated using test-tube reactions and also using n.m.r. spectroscopy.



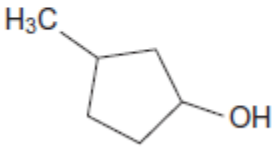
P



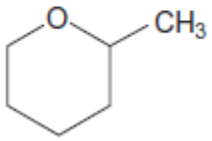
Q



R



S



T

(a) A simple test-tube reaction can be used to distinguish between isomers **P** and **S**.

Identify a reagent (or combination of reagents) you could use.
State what you would observe when both isomers are tested separately with this reagent or combination of reagents.

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(3)

(b) A simple test-tube reaction can be used to distinguish between isomer **Q** and all the other isomers.

Identify a reagent (or combination of reagents) you could use.
State what you would observe when **Q** is tested with this reagent or combination of reagents.

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(2)

(c) State which **one** of the isomers, **P**, **Q**, **R**, **S** and **T**, has the least number of peaks in its ^{1}H n.m.r. spectrum.
Give the number of peaks for this isomer.

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(2)

(d) Write the **molecular** formula of the standard used in ^{13}C n.m.r. spectroscopy.
Give **two** reasons why this compound is used.

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(3)

(e) **Figure 1** and **Figure 2** show the ^{13}C n.m.r. spectra of two of the five isomers.

Figure 1

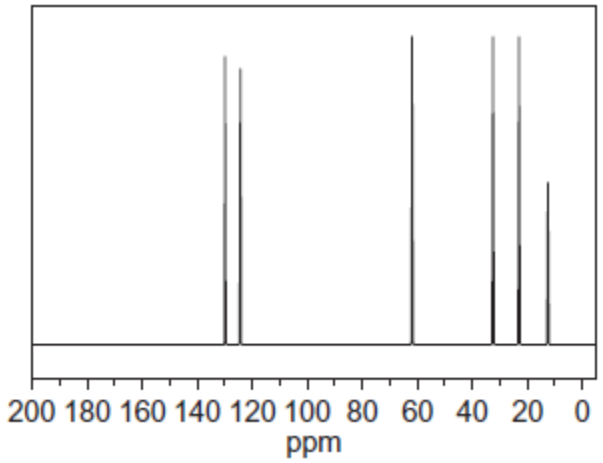
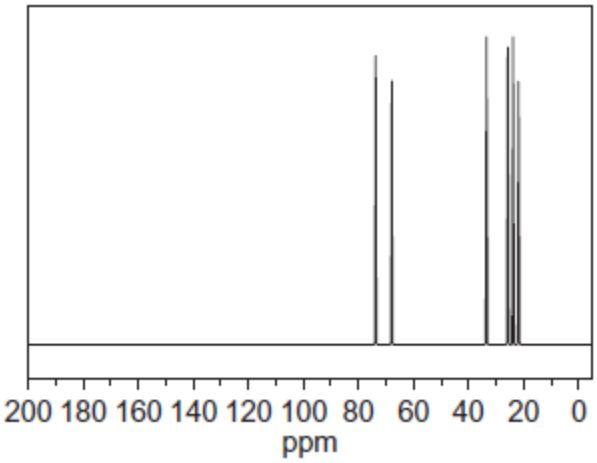
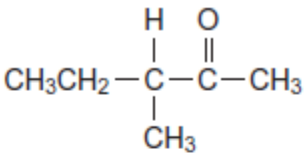


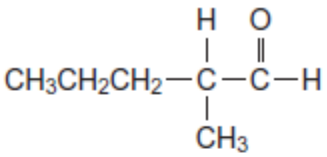
Figure 2



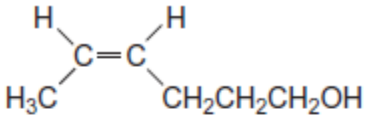
The structures of the five isomers are repeated to help you answer this question.



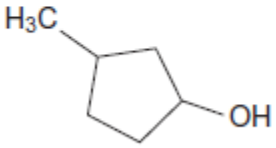
P



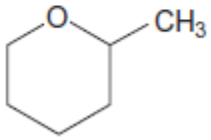
Q



R



S



T

State which isomer produces the spectrum in **Figure 1** and which isomer produces the spectrum in **Figure 2**.

Explain your answer.

You do not need to identify every peak in each spectrum.
Use **Table C** on the Data Sheet to answer the question.

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(5)

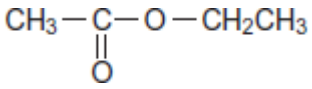
(f) **U** and **V** are other isomers of **P**, **Q**, **R**, **S** and **T**.
The ^{1}H n.m.r. spectrum of **U** consists of two singlets.
V is a cyclic alcohol that exists as optical isomers.

Draw the structure of **U** and the structure of **V**.

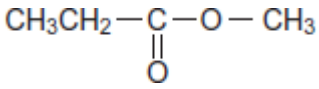
U **V**

(2)
(Total 17 marks)

5 (a) **Ester 1** and **Ester 2** were studied by ^{1}H n.m.r. spectroscopy.

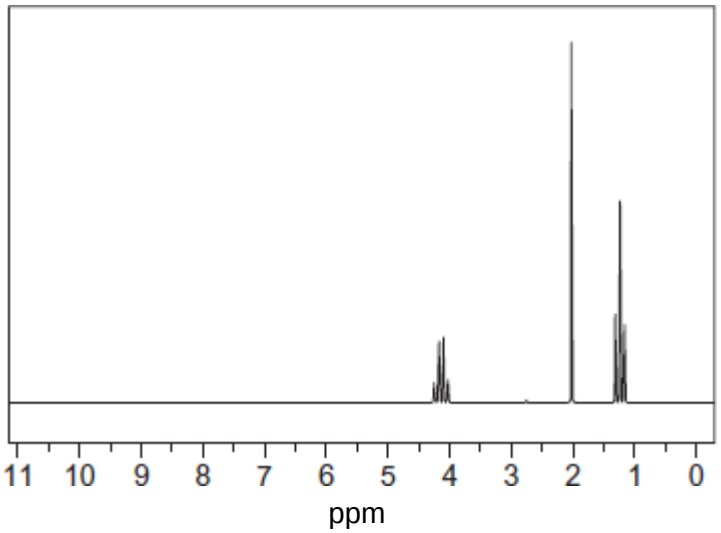


Ester 1



Ester 2

One of the two esters produced this spectrum.



Deduce which of the two esters produced the spectrum shown. In your answer, explain the position and splitting of the quartet peak at δ = 4.1 ppm in the spectrum.

Predict the δ value of the quartet peak in the spectrum of the other ester.

Use **Table B** on the Data Sheet.

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(4)

(b) Cetrimide is used as an antiseptic.

$$[CH_3(CH_2)_{15}N(CH_3)_3]^+ Br^-$$

cetrimide

Name this type of compound.

Give the reagent that must be added to $CH_3(CH_2)15NH_2$ to make cetrimide and state the reaction conditions.

Name the type of mechanism involved in this reaction.

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(4)

(c) Give a reagent that could be used in a test-tube reaction to distinguish between benzene and cyclohexene.
Describe what you would see when the reagent is added to each compound and the test tube is shaken.

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(3)
(Total 11 marks)

6 Ethanoic acid, propyl ethanoate and propan-1-ol are all colourless liquids. Esters do **not** give a positive result with any of the usual tests for functional groups.

State how you could use chemical tests to show the presence of ethanoic acid and propan-1-ol in a mixture of the acid, the alcohol and the ester.

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(Total 4 marks)

7 (a) A chemist discovered four unlabelled bottles of liquid, each of which contained a different pure organic compound. The compounds were known to be propan-1-ol, propanal, propanoic acid and 1-chloropropane.

Describe four **different** test-tube reactions, one for each compound, that could be used to identify the four organic compounds.
Your answer should include the name of the organic compound, the reagent(s) used and the expected observation for each test.

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(Extra space) .....

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(8)

(b) A fifth bottle was discovered labelled propan-2-ol. The chemist showed, using infrared spectroscopy, that the propan-2-ol was contaminated with propanone.

The chemist separated the two compounds using column chromatography. The column contained silica gel, a polar stationary phase.

The contaminated propan-2-ol was dissolved in hexane and poured into the column. Pure hexane was added slowly to the top of the column. Samples of the eluent (the solution leaving the bottom of the column) were collected.

- Suggest the chemical process that would cause a sample of propan-2-ol to become contaminated with propanone.
- State how the infrared spectrum showed the presence of propanone.
- Suggest why propanone was present in samples of the eluent collected first (those with shorter retention times), whereas samples containing propan-2-ol were collected later.

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(Extra space) .....

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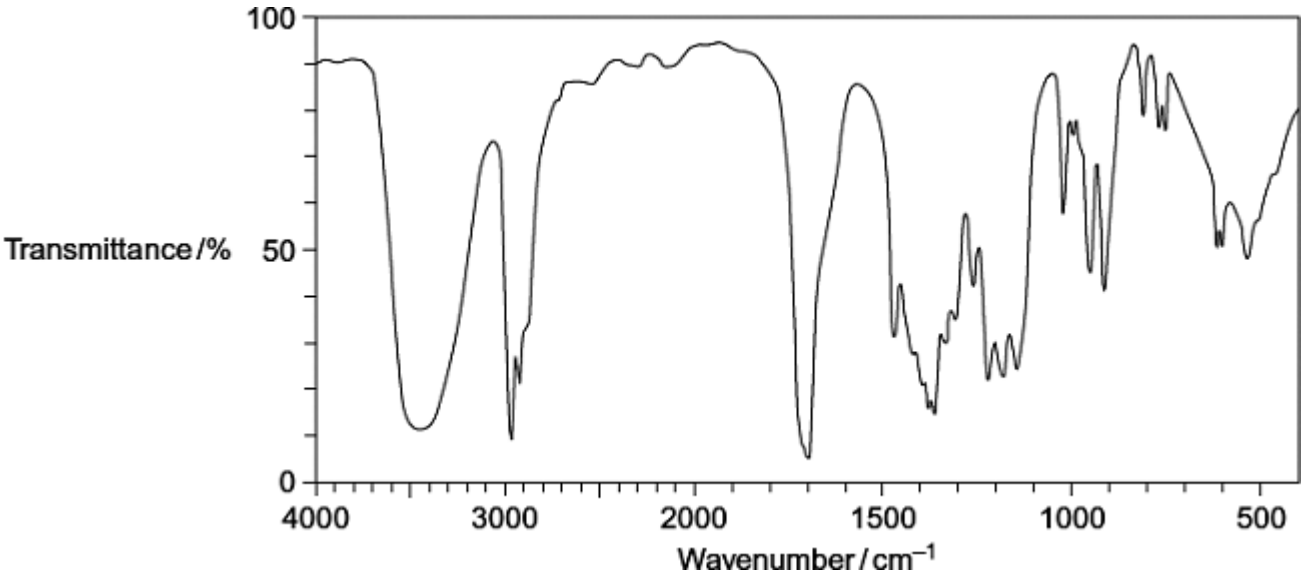
(4)
(Total 12 marks)

8 Compound **X** ($C_6H_{12}O_2$) was analysed by infrared spectroscopy and by proton nuclear magnetic resonance spectroscopy.

(a) The infrared spectrum of **X** is shown below.
Use **Table 1** on the Data Sheet to help you answer the question.



Identify the functional group that causes the absorption at 3450cm^{-1} in the spectrum.

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(1)

(b) The proton n.m.r. spectrum of **X** consists of 4 singlet peaks.

The table below gives the chemical shift for each of these peaks, together with their integration values.

δ /ppm	1.2	2.2	2.6	3.8
Integration value	6	3	2	1

Use **Table 2** on the Data Sheet to help you answer the following questions.

Use the chemical shift and the integration data to show what can be deduced about the structure of **X** from the presence of the following in its proton n.m.r. spectrum.

(i) The peak at δ = 2.6

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(1)

(ii) The peak at δ = 2.2

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(1)

(iii) The peak at δ = 1.2

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(1)

(iv) Deduce the structure of **X** ($C_6H_{12}O_2$)

(1)
(Total 5 marks)

9 (a) Propanoic acid can be made from propan-1-ol by oxidation using acidified potassium dichromate(VI). Propanal is formed as an intermediate during this oxidation.

(i) State the colour of the chromium species after the potassium dichromate(VI) has reacted.

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(1)

(ii) Describe the experimental conditions and the practical method used to ensure that the acid is obtained in a high yield. Draw a diagram of the assembled apparatus you would use.

Conditions .....

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Apparatus

(4)

(iii) Describe the different experimental conditions necessary to produce propanal in high yield rather than propanoic acid.

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(2)

(b) Propan-1-ol is a volatile, flammable liquid.
Give **one** safety precaution that should be used during the reaction to minimise this hazard.

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(1)

(c) A student followed the progress of the oxidation of propan-1-ol to propanoic acid by extracting the organic compounds from one sample of reaction mixture.

(i) Give a chemical reagent which would enable the student to confirm the presence of propanal in the extracted compounds.
State what you would observe when propanal reacts with this reagent.

Reagent .....

Observation .....

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(2)

(ii) Give a chemical reagent that would enable the student to confirm the presence of propanoic acid in the extracted compounds.
State what you would observe when propanoic acid reacts with this reagent.

Reagent .....

Observation .....

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(2)

(d) Predict which **one** of the compounds, propan-1-ol, propanal and propanoic acid will have the highest boiling point. Explain your answer.

Prediction .....

Explanation .....

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(3)
(Total 15 marks)