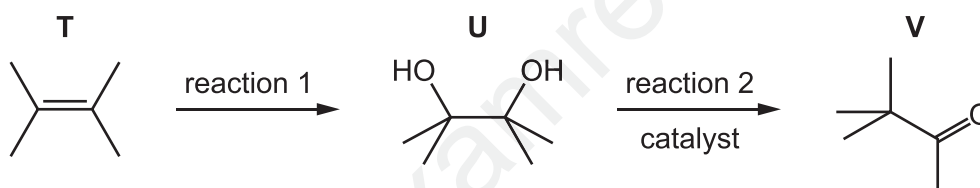


SMART EXAM RESOURCES
9701 CAMBRIDGE AS CHEMISTRY
TOPIC QUESTIONS AND MARK SCHEMES
TOPIC :ANALYTICAL TECHNIQUES
SUB-TOPIC: Analyse-Infra-red-Spectrum
SET-1-QP-MS

1 Compound **T** is an isomer of C_6H_{12} .

A reaction scheme starting with **T** is shown. Reaction 2 occurs in the presence of a catalyst; knowledge of the mechanism for this reaction is not required.



(iii) The progress of reaction 2 can be monitored by infrared spectroscopy.

The absorption caused by O–H bonds is always present because water is used as a solvent.

Identify two absorptions, and the bonds responsible for these absorptions, whose appearance will change significantly during the reaction.

1

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2

.....

[2]

MARK SCHEME:

(iii)	M1 C—O in range 1040–1300 (cm ⁻¹)	2
	M2 C=O in range 1670–1740 (cm ⁻¹)	

- 2 Lactones are cyclic esters. Under suitable conditions, lactones form from molecules that have both an alcohol and a carboxylic acid functional group.
Equation 1 shows an example of the formation of a lactone.

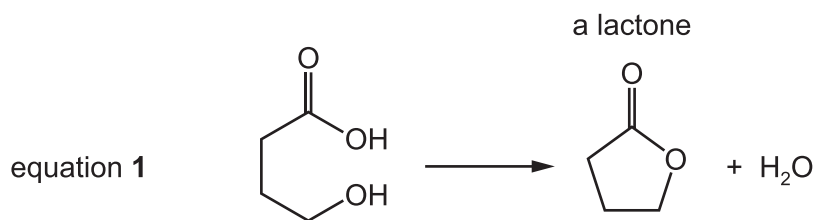


Fig. 5.1 shows the synthesis of lactone **P** from compound **M**.

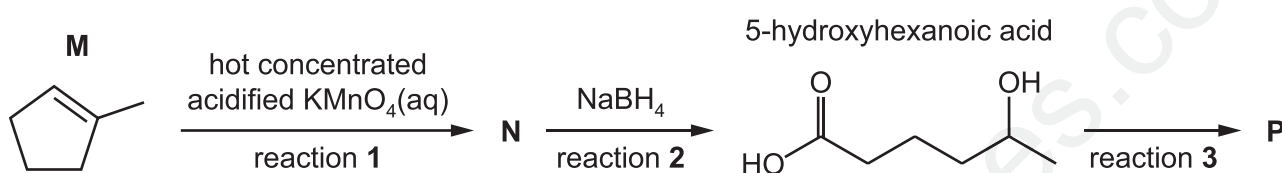


Fig. 5.1

- (a) (i) **M** reacts with hot concentrated acidified $\text{KMnO}_4(\text{aq})$ to form **N**, $\text{C}_6\text{H}_{10}\text{O}_3$, in reaction 1.

Draw the structure of **N**.

[1]

- (ii) **N** is reduced by NaBH_4 to form 5-hydroxyhexanoic acid in reaction 2.

Construct an equation for reaction 2 using molecular formulae.

In the equation, use $[\text{H}]$ to represent one atom of hydrogen from the reducing agent.

..... [1]

- (iii) Reaction 2 is a nucleophilic addition.

Suggest why reaction 2 creates a mixture of two organic compounds.

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..... [2]

(iv) Draw lactone **P**, the product of reaction **3**.

[1]

(b) A student monitors the progress of reaction **2** using infrared spectroscopy.

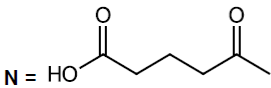
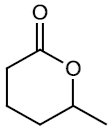
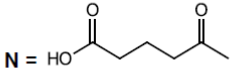
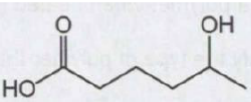
Use Table 5.1 to suggest why it is difficult to distinguish between **N** and 5-hydroxyhexanoic acid using infrared spectroscopy.

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 [2]

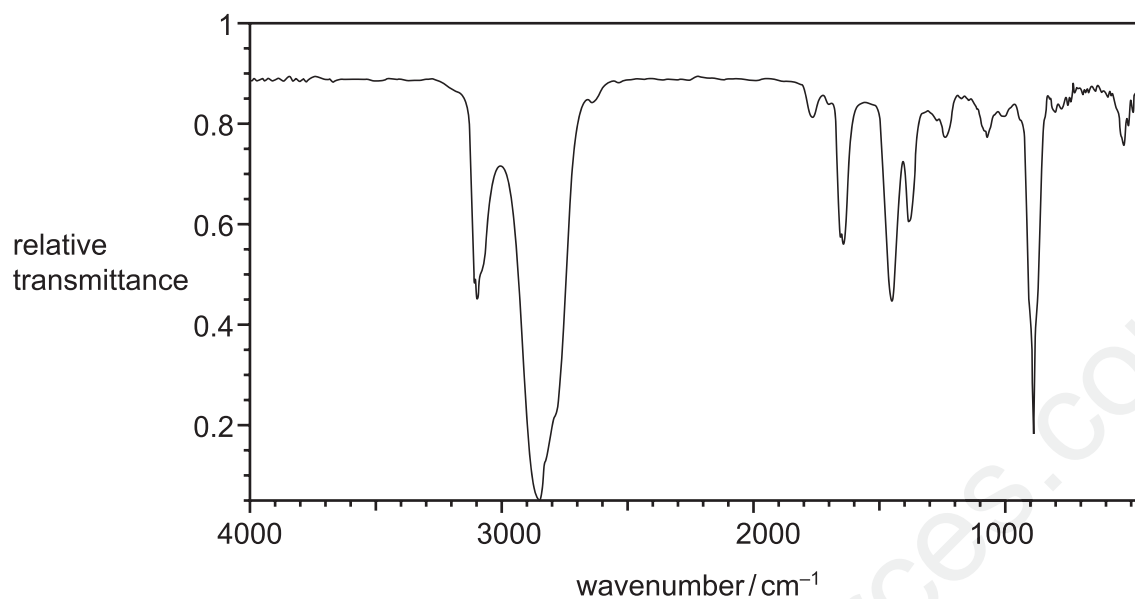
Table 5.1

bond	functional group containing the bond	characteristic infrared absorption range (in wavenumbers)/cm ⁻¹
C–O	hydroxy, ester	1040–1300
C=C	aromatic compound, alkene	1500–1680
C=O	amide carbonyl, carboxyl ester	1640–1690 1670–1740 1710–1750
C≡N	nitrile	2200–2250
C–H	alkane	2850–3100
N–H	amine, amide	3300–3500
O–H	carboxyl hydroxy	2500–3000 3200–3650

MARK SCHEME:

(a)(i)	 <chem>CC(=O)CCCC(=O)O</chem>	1
(a)(ii)	$C_6H_{10}O_3 + 2[H] \rightarrow C_6H_{12}O_3$	1
(a)(iii)	M1 (ketone in) N is planar (so can be attacked from either side)	1
	M2 because different stereoisomers / optical isomers form	1
(a)(iv)		1
(b)	<div>  ; 5-hh  </div> <hr/> M1 absorptions will overlap / be similar / the same / indistinguishable	1

3 The infra-red spectrum of 2-methylbut-1-ene is shown.



Predict two main differences that would be seen between the spectra of **Y**, $\text{CH}_3\text{CH}_2\text{COCH}_3$, and of 2-methylbut-1-ene. Give reasons for your predictions.

Your answer should refer only to the region of each spectrum **above 1500 cm⁻¹**.

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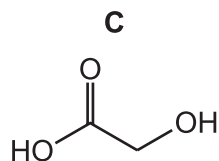
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..... [2]

MARK SCHEME:

<p>Predict two differences, with reasons, between spectra of Y, $\text{CH}_3\text{CH}_2\text{COCH}_3$ and 2-methylbut-1-ene (shown)</p> <p><i>first difference</i></p> <p>M1 absence of peak/ absorption at $3100\text{ (cm}^{-1}\text{)}$ as no longer any =C-H present (in Y)</p> <p><i>second difference</i></p> <p>M2 peak at $1650\text{ (cm}^{-1}\text{)}$ moves to the left to any value / range of values between 1670 and 1740) due to disappearance of C=C (in Y) and appearance of C=O (in Y)</p> <p>OR</p> <p>absence of peak at $1650\text{ (cm}^{-1}\text{)}$ as no longer any C=C present (in Y)</p> <p>AND</p> <p>appearance of peak (in Y) at (any value / range of values) between $1670\text{-}1740\text{(cm}^{-1}\text{)}$ due to C=O</p>	2
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4 Reaction 2 needs to take place in the absence of water to prevent formation of compound **C**.



If **C** is present in the reaction mixture of reaction 3, a different compound, compound **D**, will also form. Compound **D** has two identical functional groups.

The infrared spectrum of **D** shows strong absorptions at 1100 cm^{-1} and 1720 cm^{-1} , but no absorption due to O–H bonds.

Use the *Data Booklet* to identify the functional group present in **D**.

Explain your answer as fully as you can.

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..... [3]

MARK SCHEME:

M1 ester	3
M2 1100 cm ⁻¹ linked to C—O AND 1720 cm ⁻¹ linked to C=O	
M3 No COOH / carboxylic acid and No OH / alcohol in D (but present in C)	
OR	
COOH / carboxylic acid and OH / alcohol reacted /lost (in C to form D)	

- 5 Propanone, CH_3COCH_3 , is an important organic reagent. Fig. 4.1 shows some reactions of propanone and its derivatives.

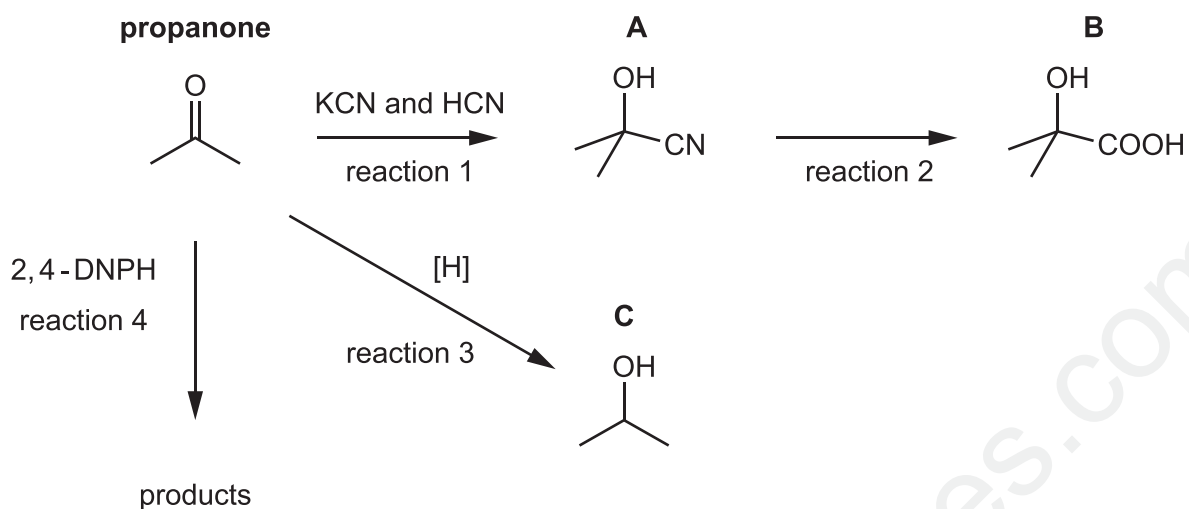


Fig. 4.1

(f) Compounds **A**, **B** and **C** can be distinguished using infrared spectroscopy.

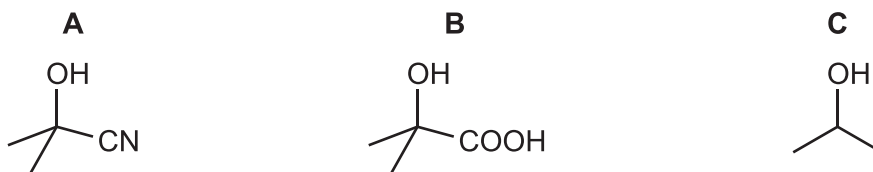


Fig. 4.3 shows the infrared spectrum of one of the compounds.

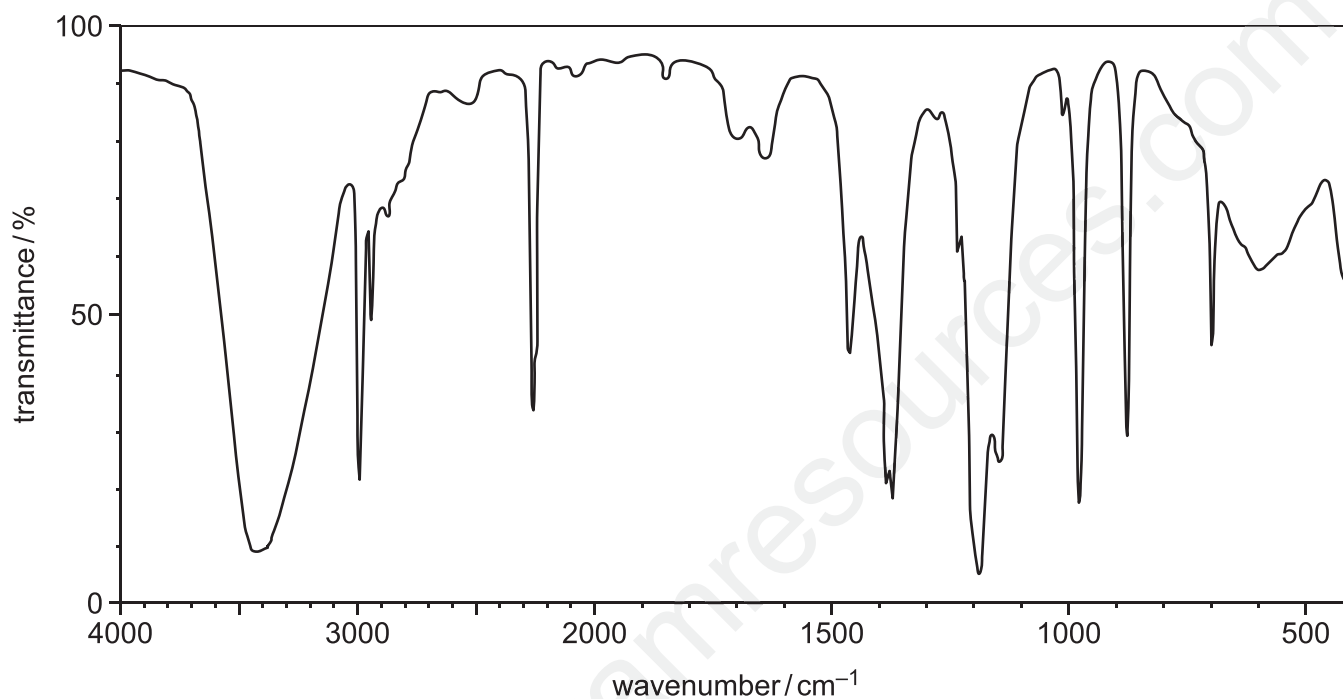


Fig. 4.3

Table 4.1

bond	functional groups containing the bond	characteristic infrared absorption range (in wavenumbers)/cm ⁻¹
C—O	hydroxy, ester	1040–1300
C=C	aromatic compound, alkene	1500–1680
C=O	amide carbonyl, carboxyl ester	1640–1690 1670–1740 1710–1750
C≡N	nitrile	2200–2250
C—H	alkane	2850–2950
N—H	amine, amide	3300–3500
O—H	carboxyl hydroxy	2500–3000 3200–3600

- (i) Explain why the absorptions at $2850\text{--}2950\text{ cm}^{-1}$ are **not** useful to help determine which of the compounds **A**, **B** or **C** produces the infrared spectrum in Fig. 4.3.

Use Table 4.1 to answer this question.

.....

..... [1]

- (ii) Identify which of compounds **A**, **B** or **C** produces the infrared spectrum in Fig. 4.3. Explain your answer.

compound

explanation

.....

.....

[1]

Mark Scheme:

(f)(i)	All three have a C—H OR CH bond	1
(f)(ii)	compound A AND absorption at 2200–2250 cm ⁻¹ indicates C≡N	1