22. Analytical techniques

22.1 Infrared spectroscopy

Paper 2

Question Paper

1 **(c)** Both functional groups in one molecule of **Y** react with an inorganic reagent to form one molecule of **Q** and one molecule of methanol, CH_3OH, as shown in Fig. 6.3.

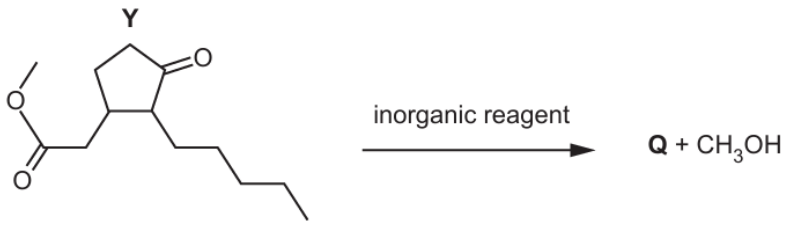

Fig. 6.3

(i) Part of the mass spectrum for **Q** is shown in Fig. 6.4. Only peaks with *m*/*e* greater than 198 are shown.

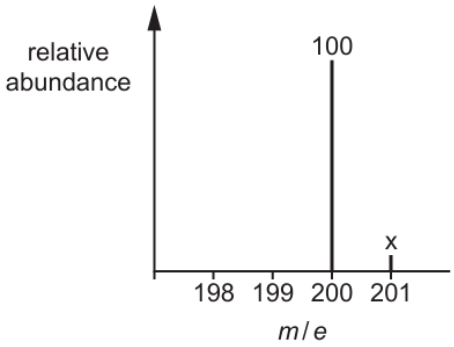

Fig. 6.4

Calculate the relative abundance, x, of the peak at *m*/*e* = 201.

Show your working.

x = ... [2]

(ii) **Q** contains **only** hydroxyl functional groups.

Complete Table 6.1 to show the observations that occur when 2,4-dinitrophenylhydrazine (2,4-DNPH reagent) is added to separate samples of **Y** and **Q**.

Table 6.1

	observation on addition of 2,4-DNPH reagent
Y	
Q	

[1]

(iii) Under certain conditions, 0.0020 mol of **Q** reacts with an excess of sodium to produce a total of 44.8 cm^3 of gas at s.t.p.

Calculate the number of hydroxyl groups present in a molecule of **Q**.

Show your working.

number of hydroxyl groups = ... [2]

(iv) Use Table 6.2 to describe and explain **two** differences between the infrared spectrum of **Y** and **Q** in the region above 1500 cm^{-1}.

.....

.....

..... [2]

Table 6.2

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 3200–3650

2 **(b)** A sample of **W**, $C_4H_{10}O$, is heated under reflux with an excess of acidified $K_2Cr_2O_7$ until there is no further reaction. Only **one** organic product, **X**, is present in the mixture at the end of the reaction.

Fig. 5.1 shows the infrared spectrum of **W**.

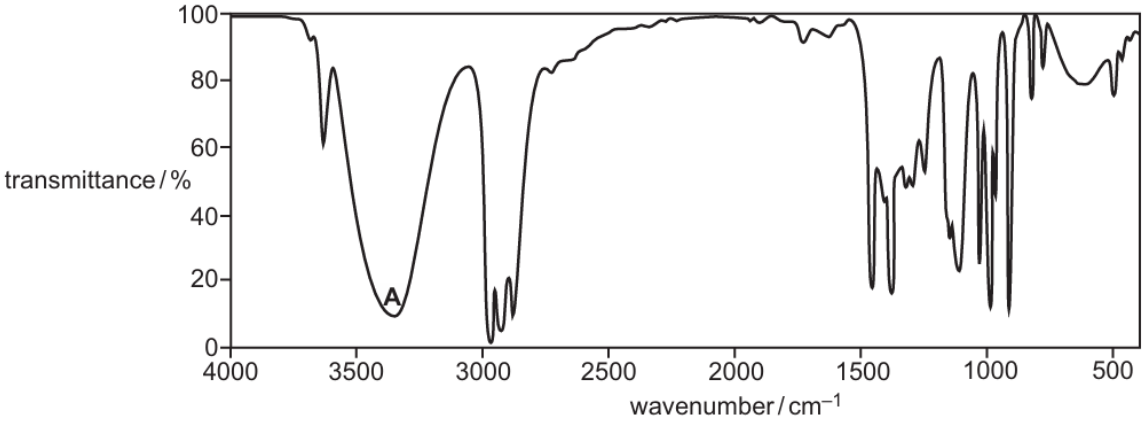

Fig. 5.1

Fig. 5.2 shows the infrared spectrum of **X**.

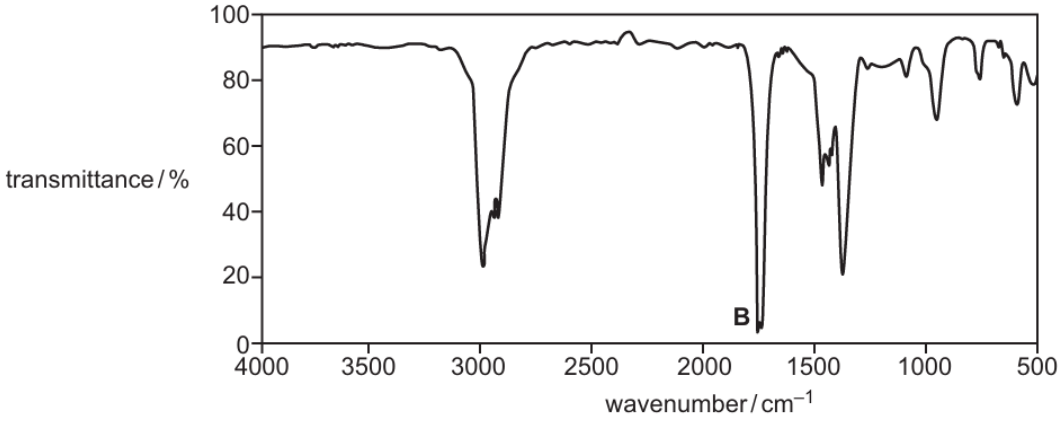

Fig. 5.2

Table 5.2

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 3200–3650

(i) Absorption **A** is shown in Fig. 5.1.
Absorption **B** is shown in Fig. 5.2.

Complete Table 5.3 using the information given in Fig. 5.1, Fig. 5.2 and Table 5.2.

Table 5.3

absorption	bond	functional group containing the bond
A		
B		

[1]

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

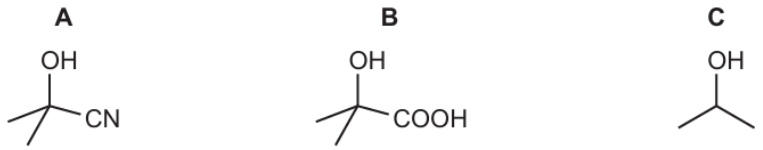

Fig. 4.3 shows the infrared spectrum of one of the compounds.

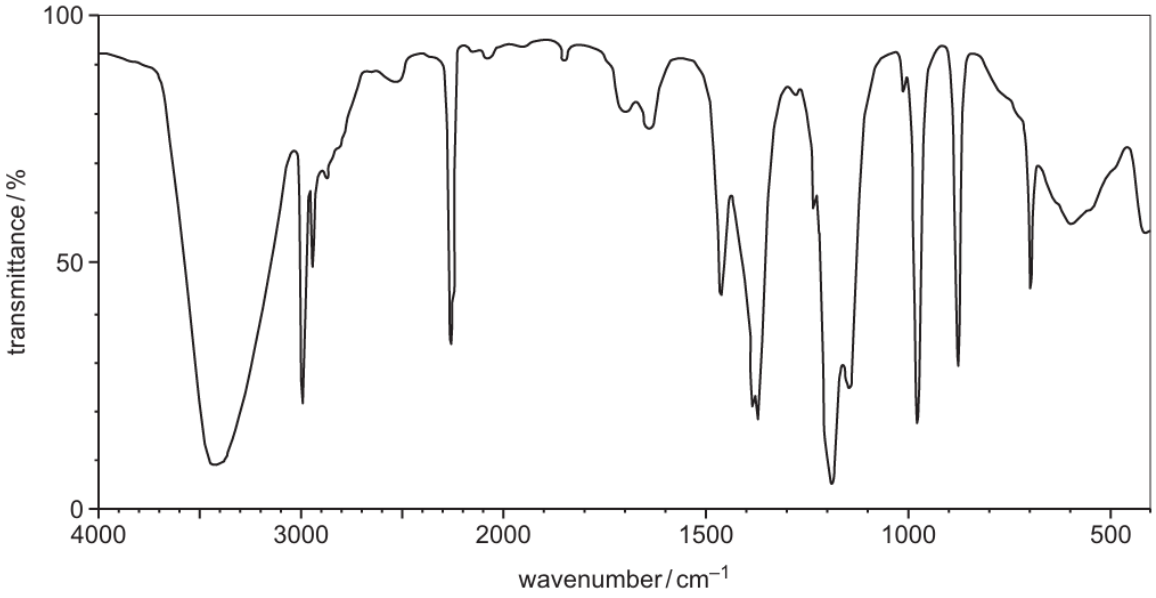

Fig. 4.3

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 2850–2950 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]

4 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.

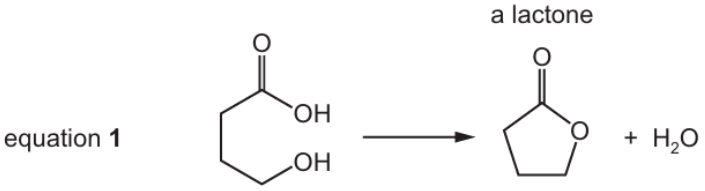

Fig. 5.1 shows the synthesis of lactone **P** from compound **M**.

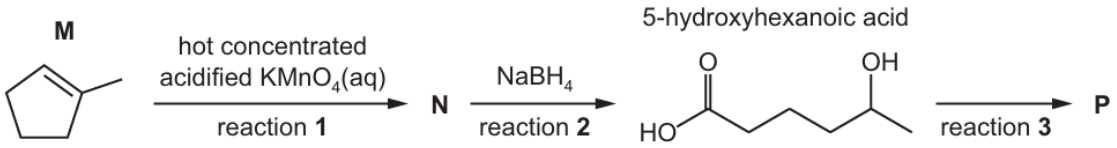

Fig. 5.1

(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.

.....

..... [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

5 **(c)** Organic compound **E** contains three carbon atoms.
E reacts with cold dilute acidified $KMnO_4(aq)$ to form a single compound **F** with M_r = 154.9.
Fig. 3.1 shows the infrared spectrum of **E**.
Fig. 3.2 shows the infrared spectrum of **F**.

E

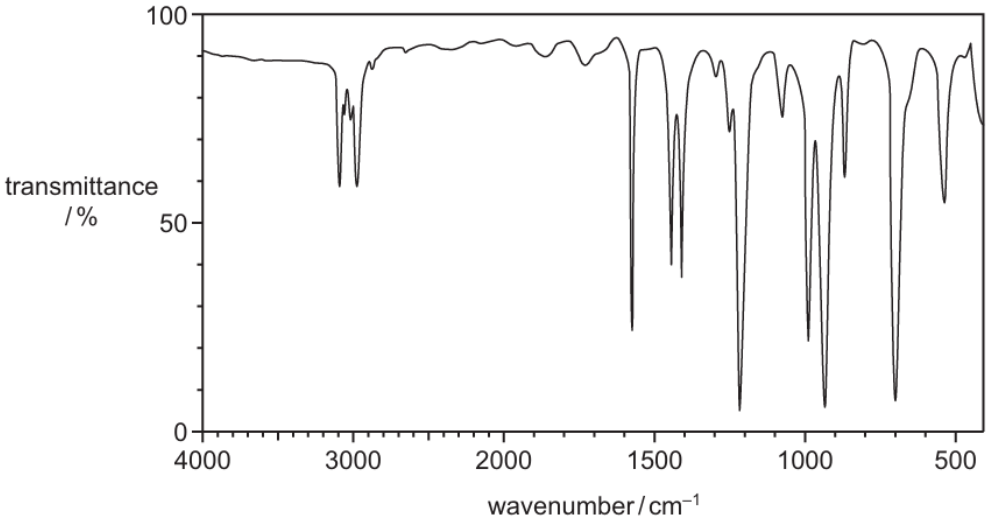

Fig. 3.1

F

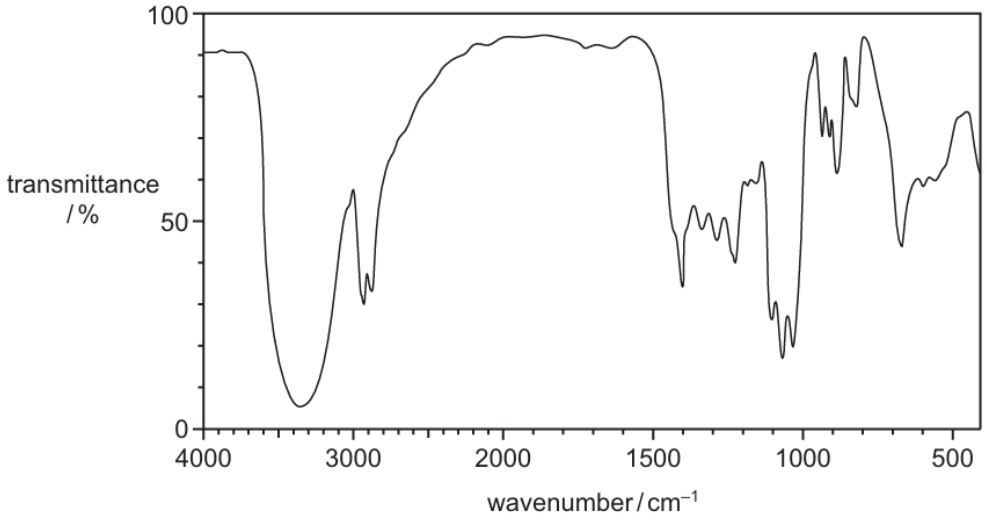

Fig. 3.2

Table 3.2

bond	functional group containing the bond	characteristic infrared absorption range (in wavenumbers) / cm^{-1}
C–O	hydroxy, ester	1040–1300
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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

Both spectra show absorptions between 2850 and 2950 cm^{-1} owing to C–H bonds in each molecule.

(i) Use the two infrared spectra and Table 3.2 to identify the functional group present only in **E**.
Explain your answer, referring only to absorptions at frequencies greater than 1500 cm^{-1}.

functional group .....

explanation .....

.....
[1]

(ii) Use the infrared spectrum of **F** to identify the functional group formed when **E** reacts with cold dilute acidified $KMnO_4(aq)$.
Explain your answer, referring only to absorptions at frequencies greater than 1500 cm^{-1}.

functional group .....

explanation .....

.....
[1]

(iii) The mass spectrum of **E** shows a molecular ion peak and an M+2 peak of approximately equal abundance at m/e = 120 and 122.

Deduce the relative molecular mass, M_r, of **E**.

M_r = ... [1]

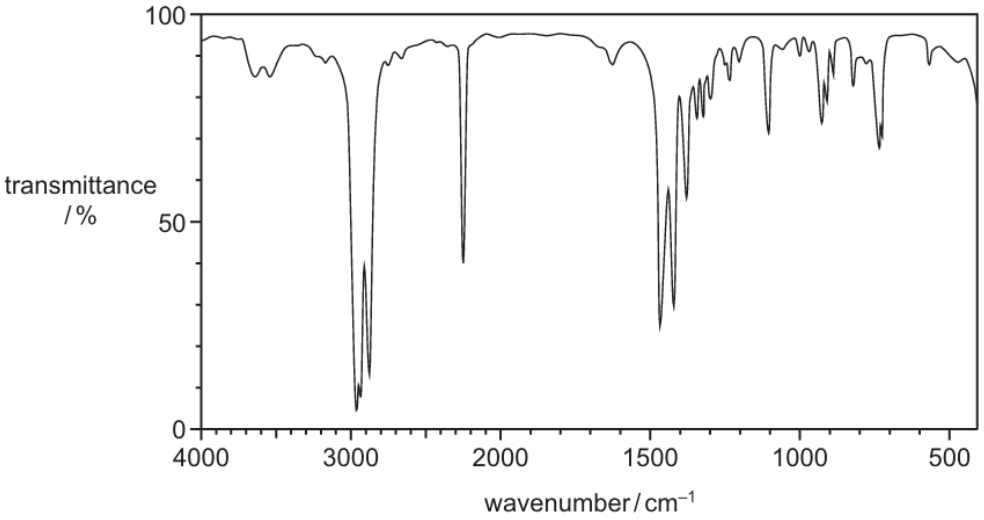
6 **S** is a secondary alcohol with molecular formula $C_4H_{10}O$.

(b) **S** is converted to **V** in a three-step reaction sequence.

In step 1, the secondary alcohol **S** reacts with PBr_3 to produce **T**, which has molecular formula C_4H_9Br.

(v) An unlabelled sample contains either **S**, **T** or **U**.

The sample produces the infrared spectrum shown.



Explain how this spectrum confirms that the unknown sample contains **U**.

In your answer identify **one** relevant absorption in the infrared spectrum and the bond that corresponds to this absorption in the region above 1500 cm^{-1}.

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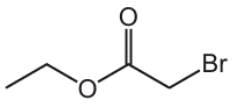
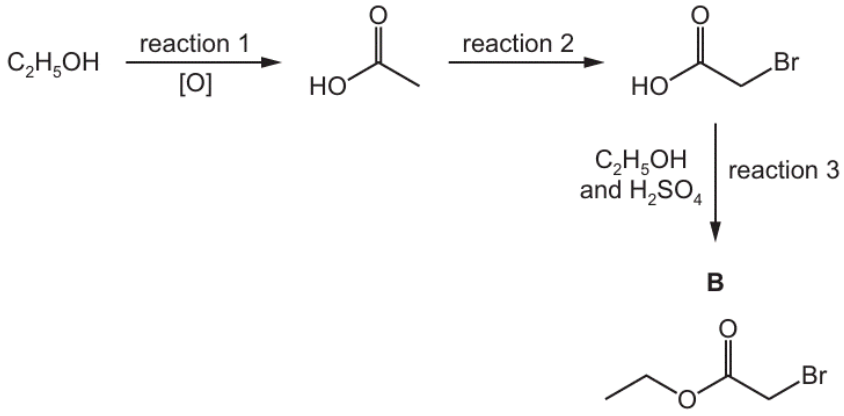
..... [1]

7 Compound **B** is a liquid with a fruity smell.

B



The reaction scheme shows how **B** can be made from ethanol, C_2H_5OH.



(a) (i) Reaction 1 is an oxidation reaction.

Give the reagent(s) and conditions required for reaction 1.

reagent(s) .....

conditions .....

.....

[2]

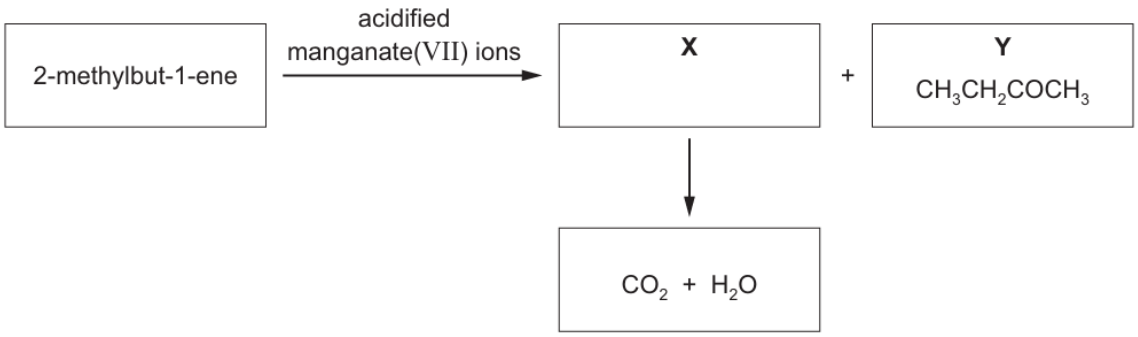
(ii) Construct an equation to represent reaction 1.

Use [O] to represent an oxygen atom from the oxidising agent in this reaction.

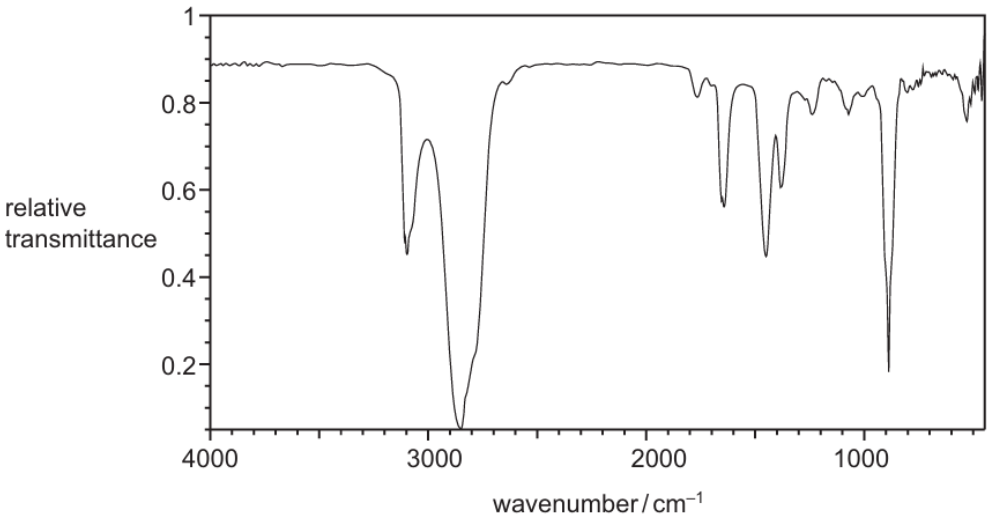
..... [1]

8 2-methylbut-1-ene reacts with acidified manganate(VII) ions, under specific conditions, to produce two organic compounds **X** and **Y**.

X immediately reacts with the acidified manganate(VII) ions to form carbon dioxide and water. **Y** has the structural formula $CH_3CH_2COCH_3$.



(e) The infra-red spectrum of 2-methylbut-1-ene is shown.



Predict two main differences that would be seen between the spectra of **Y**, $CH_3CH_2COCH_3$, 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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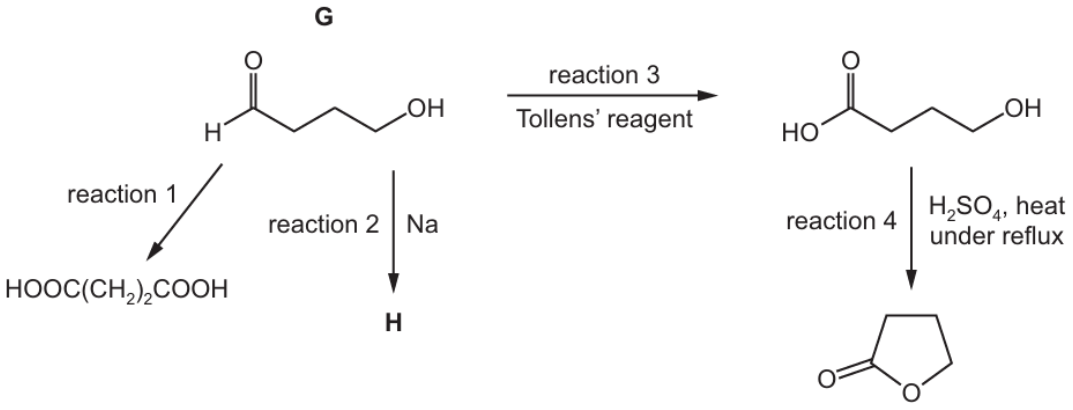
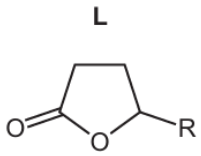
..... [2]

9 Some reactions of compound **G** are shown.

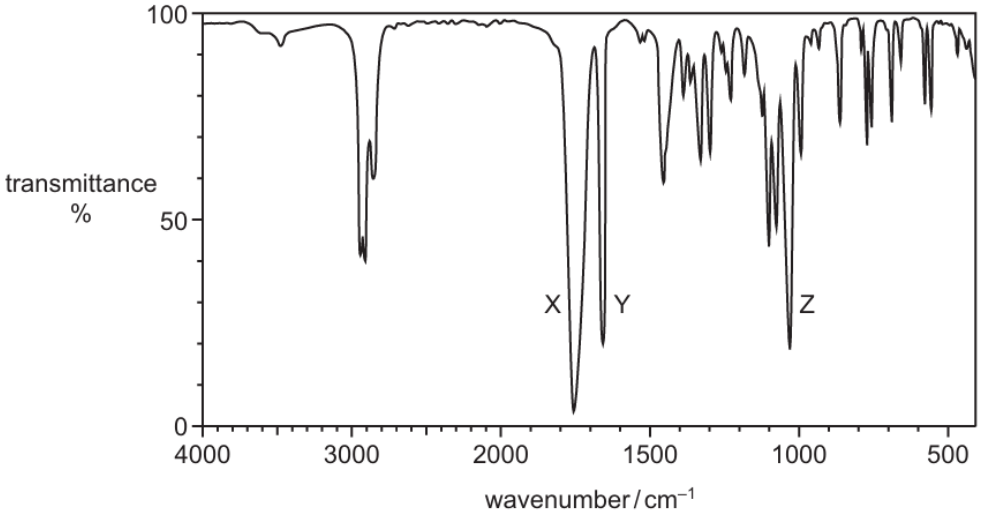


(d) The structure of compound **L** is shown. R represents a hydrocarbon chain.



A student was asked to deduce the full structure of **L**.

The student analysed **L** using infrared spectroscopy. The following spectrum was obtained.



(i) Identify the bonds responsible for the absorptions marked X and Z.

X .....

Z .....

[1]