

40 The purity of a compound can be determined using infrared spectroscopy.

The table gives the characteristic infrared absorption frequencies for some selected bonds.

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

Propan-2-ol is made by hydration of propene. A sample of the product is obtained.

Which feature of the infrared spectrum of the product would show that **no** propene remains in the product?

- A absorption in the 2900 cm⁻¹ region
- B strong absorption below 1000 cm⁻¹
- C the lack of absorption at or near 1250 cm⁻¹
- D the lack of absorption at or near 1550 cm⁻¹

Important values, constants and standards

molar gas constant	$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
Faraday constant	$F = 9.65 \times 10^4 \text{ C mol}^{-1}$
Avogadro constant	$L = 6.02 \times 10^{23} \text{ mol}^{-1}$
electronic charge	$e = -1.60 \times 10^{-19} \text{ C}$
molar volume of gas	$V_m = 22.4 \text{ dm}^3 \text{ mol}^{-1}$ at s.t.p. (101 kPa and 273 K) $V_m = 24.0 \text{ dm}^3 \text{ mol}^{-1}$ at room conditions
ionic product of water	$K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$ (at 298 K (25 °C))
specific heat capacity of water	$c = 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ (4.18 J g ⁻¹ K ⁻¹)

The Periodic Table of Elements

Group																	
1	2	Key														18	
3	4	atomic number atomic symbol name relative atomic mass														2	
Li lithium 6.9	Be beryllium 9.0															He helium 4.0	
11	12																
Na sodium 23.0	Mg magnesium 24.3																
19	20																
K potassium 39.1	Ca calcium 40.1																
37	38																
Rb rubidium 85.5	Sr strontium 87.6																
55	56																
Cs caesium 132.9	Ba barium 137.3																
87	88																
Fr francium —	Ra radium —																
57	58																
La lanthanum 138.9	Ce cerium 140.1																
89	90																
Ac actinium —	Th thorium 232.0																
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- 4 Fig. 4.1 shows how propane, C_3H_8 , can be converted to propanoic acid, CH_3CH_2COOH .

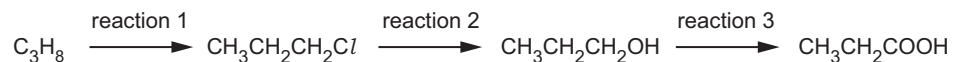
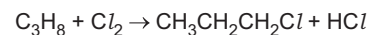


Fig. 4.1

- (a) Reaction 1 in Fig. 4.1 takes place in the presence of sunlight.



The reaction takes place via initiation, propagation and termination steps.

- (i) Name the mechanism shown by reaction 1.

..... [1]

- (ii) Complete the mechanism for reaction 1.

Construct equations to describe the steps of the mechanism.



propagation 1

propagation 2

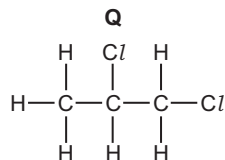
termination $\rightarrow CH_3CH_2CH_2Cl$
[3]

- (iii) Reaction 1 is initiated by the bond fission of Cl_2 .

State the type of bond fission shown in the initiation step.

..... [1]

- (iv) Compound **Q** is a by-product of reaction 1.



Name **Q**.

..... [1]

- (v) The molecular formula of **Q** is $C_3H_6Cl_2$.

Identify the types of structural isomerism and stereoisomerism that a molecule with molecular formula $C_3H_6Cl_2$ can show.

type of structural isomerism

type of stereoisomerism [2]

- (b) State the reagent and solvent required for reaction 2.

..... [1]

- (c) Reaction 3 takes place when $CH_3CH_2CH_2OH$ is heated under reflux with acidified potassium dichromate(VI) solution.

- (i) State the colour change that takes place in the reaction mixture.

..... [1]

- (ii) Construct an equation to represent reaction 3. Use [O] to represent an atom of oxygen from the oxidising agent.

..... [1]

(d) $\text{CH}_3\text{CH}_2\text{COOH}$ reacts with an unsaturated alcohol **R** to form unsaturated ester **S**.

(i) State the **type** of reaction that forms **S**.

..... [1]

(ii) The infrared spectrum of **S** is shown in Fig. 4.2.

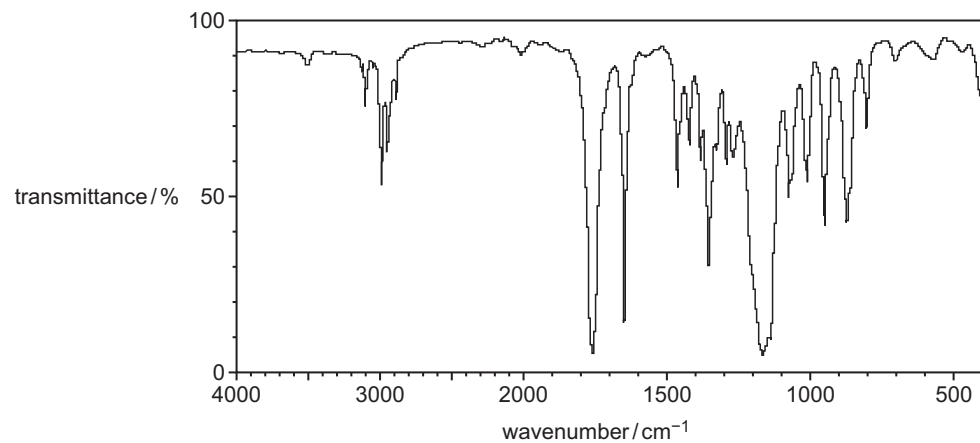


Fig. 4.2

Three absorptions in the infrared spectrum in Fig. 4.2 confirm that **S** is an ester and is unsaturated.

- Write **1**, **2** or **3** on Fig. 4.2 against each of these three absorptions.
- Complete Table 4.1 to show which bond is responsible for each absorption that you have identified in Fig. 4.2.

Table 4.1

absorption	1	2	3
bond responsible			

[3]

Table 4.2

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

(iii) The mass spectrum of **S** shows the following peaks.

Table 4.3

peak	relative abundance
M^+	4.7
$[\text{M}+1]^+$	0.31

Use Table 4.3 to calculate the number of carbon atoms in **S**.

number of carbon atoms in **S** = [1]

[Total: 16]

⑦

molar gas constant	$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$
Faraday constant	$F = 9.65 \times 10^4 \text{ C mol}^{-1}$
Avogadro constant	$L = 6.02 \times 10^{23} \text{ mol}^{-1}$
electronic charge	$e = -1.60 \times 10^{-19} \text{ C}$
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specific heat capacity of water	$c = 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$ ($4.18 \text{ J g}^{-1} \text{ K}^{-1}$)

The Periodic Table of Elements

Group																
										1						
										H						
										hydrogen						
										1.0						

lanthanoids

57	La	58	Ce	59	Pr	60	Nd	61	Pm	62	Sm	63	Eu	64	Gd	65	Tb	66	Dy	67	Ho	68	Er	69	Tm	70	Yb	71	Lu
lanthanum		cerium		praseodymium		neodymium		promethium		samarium		euroium		gadolinium		terbium		dysprosium		holmium		erbium		thulium		ytterbium		lutetium	
138.9		140.1		140.9		144.2		—		150.4		152.0		157.3		162.5		162.5		164.9		167.3		168.9		173.1		175.0	
89	Ac	90	Th	91	Pa	92	U	93	Np	94	Pu	95	Am	96	Cm	97	Bk	98	Cf	99	Es	100	Fm	101	Md	102	No	103	Lr
actinium		thorium		protactinium		uranium		neptunium		plutonium		americium		curium		berkelium		californium		einsteinium		fermium		mendelevium		nobelium		lawrencium	

actinoids