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}

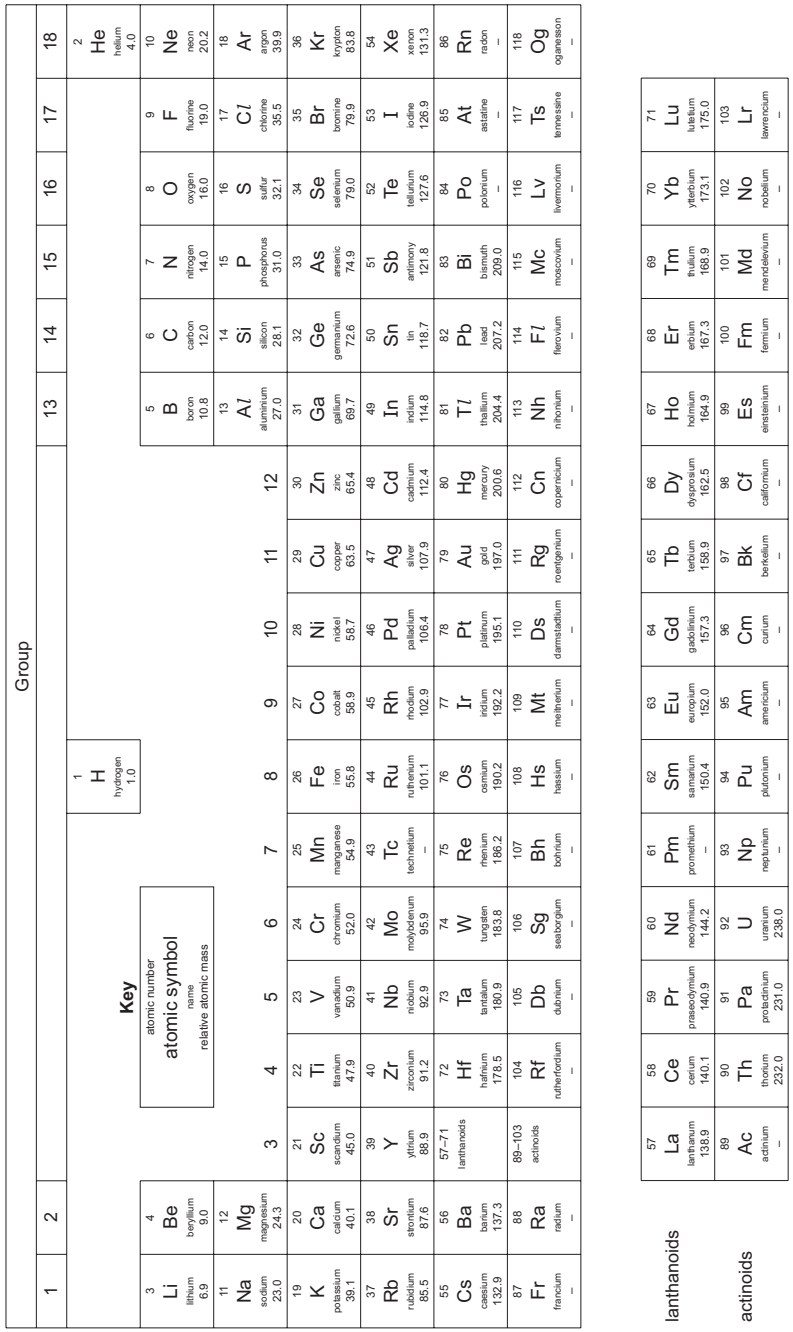
C the lack of absorption at or near 1250 cm^{-1}

D the lack of absorption at or near 1550 cm^{-1}

Important values, constants and standards

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

The Periodic Table of Elements



4 Fig. 4.1 shows how propane, C_3H_8, can be converted to propanoic acid, CH_3CH_2COOH.

$$C_3H_8 \xrightarrow{\text{reaction 1}} CH_3CH_2CH_2Cl \xrightarrow{\text{reaction 2}} CH_3CH_2CH_2OH \xrightarrow{\text{reaction 3}} CH_3CH_2COOH$$

Fig. 4.1

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

$$C_3H_8 + Cl_2 \rightarrow CH_3CH_2CH_2Cl + HCl$$

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.

initiation $Cl_2 \rightarrow 2Cl\bullet$

propagation 1 .....

propagation 2 .....

termination ..... $\rightarrow CH_3CH_2CH_2Cl$ [3]

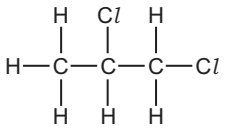
(iii) Reaction 1 is initiated by the bond fission of Cl_2.

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

..... [1]

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

Q



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) CH_3CH_2COOH 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.

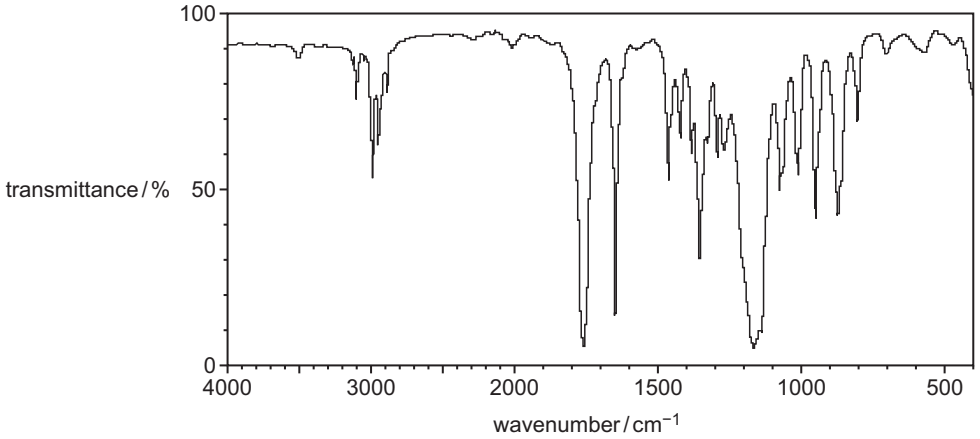


Fig. 4.2

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
$[M+1]^+$	0.31

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

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

[Total: 16]

Important values, constants and standards

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

The Periodic Table of Elements

Group																	
1	2											13	14	15	16	17	18
							1 H hydrogen 1.0										2 He helium 4.0
3 Li lithium 6.9	4 Be beryllium 9.0											5 B boron 10.8	6 C carbon 12.0	7 N nitrogen 14.0	8 O oxygen 16.0	9 F fluorine 19.0	10 Ne neon 20.2
11 Na sodium 23.0	12 Mg magnesium 24.3	3	4	5	6	7	8	9	10	11	12	13 Al aluminium 27.0	14 Si silicon 28.1	15 P phosphorus 31.0	16 S sulfur 32.1	17 Cl chlorine 35.5	18 Ar argon 39.9
19 K potassium 39.1	20 Ca calcium 40.1	21 Sc scandium 45.0	22 Ti titanium 47.9	23 V vanadium 50.9	24 Cr chromium 52.0	25 Mn manganese 54.9	26 Fe iron 55.8	27 Co cobalt 58.9	28 Ni nickel 58.7	29 Cu copper 63.5	30 Zn zinc 65.4	31 Ga gallium 69.7	32 Ge germanium 72.6	33 As arsenic 74.9	34 Se selenium 79.0	35 Br bromine 79.9	36 Kr krypton 83.8
37 Rb rubidium 85.5	38 Sr strontium 87.6	39 Y yttrium 88.9	40 Zr zirconium 91.2	41 Nb niobium 92.9	42 Mo molybdenum 95.9	43 Tc technetium –	44 Ru ruthenium 101.1	45 Rh rhodium 102.9	46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	49 In indium 114.8	50 Sn tin 118.7	51 Sb antimony 121.8	52 Te tellurium 127.6	53 I iodine 126.9	54 Xe xenon 131.3
55 Cs caesium 132.9	56 Ba barium 137.3	57–71 lanthanoids	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.8	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 192.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.6	81 Tl thallium 204.4	82 Pb lead 207.2	83 Bi bismuth 209.0	84 Po polonium –	85 At astatine –	86 Rn radon –
87 Fr francium –	88 Ra radium –	89–103 actinoids	104 Rf rutherfordium –	105 Db dubnium –	106 Sg seaborgium –	107 Bh bohrium –	108 Hs hassium –	109 Mt meitnerium –	110 Ds darmstadtium –	111 Rg roentgenium –	112 Cn copernicium –	113 Nh nihonium –	114 Fl flerovium –	115 Mc moscovium –	116 Lv livermorium –	117 Ts tennessine –	118 Og oganesson –

Key

atomic number
atomic symbol
name
relative atomic mass

lanthanoids	57 La lanthanum 138.9	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium –	62 Sm samarium 150.4	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.1	71 Lu lutetium 175.0
actinoids	89 Ac actinium –	90 Th thorium 232.0	91 Pa protactinium 231.0	92 U uranium 238.0	93 Np neptunium –	94 Pu plutonium –	95 Am americium –	96 Cm curium –	97 Bk berkelium –	98 Cf californium –	99 Es einsteinium –	100 Fm fermium –	101 Md mendelevium –	102 No nobelium –	103 Lr lawrencium –