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

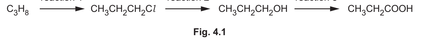


Fig. 4.1

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

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

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.

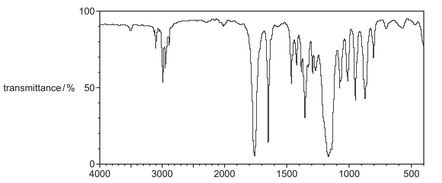


Fig. 4.2

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

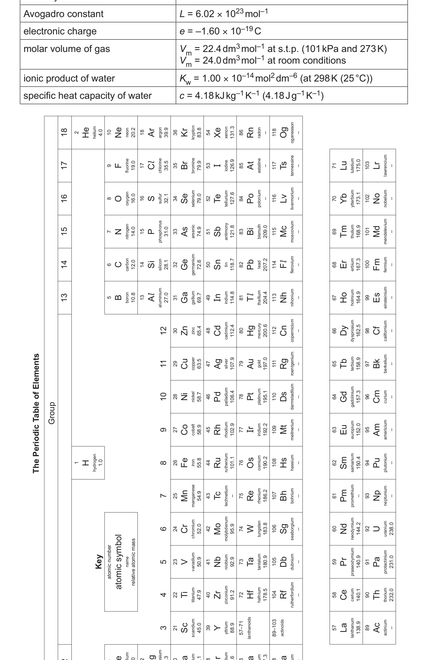
peak	relative abundance
M^+	4.7
$[M+1]^+$	0.31

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	$c = 4.18\,kJ\,kg^{-1}\,K^{-1}$ ($4.18\,J\,g^{-1}\,K^{-1}$)