22. Analytical techniques

22.2 Mass spectrometry

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.

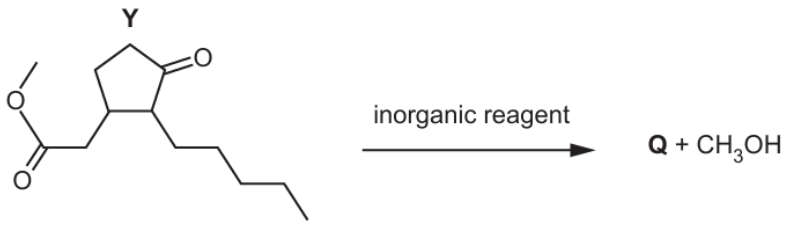


Fig. 6.3

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

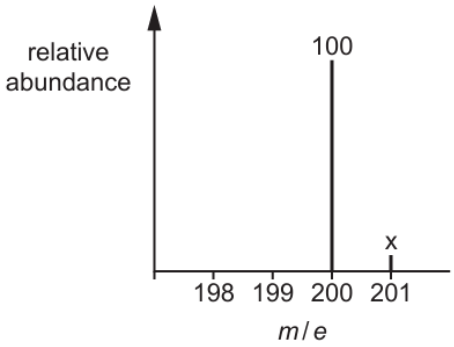


Fig. 6.4

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

Show your working.

x = ... [2]

2 Compound **W** has molecular formula $C_4H_{10}O$. It contains only **one** functional group.

(a) Table 5.1 shows the two peaks with the greatest *m*/*e* values in the mass spectrum of **W**.

Table 5.1

m/*e*	relative abundance
74	50
75	x

(i) Calculate the relative abundance, x, of the peak at *m*/*e* = 75 using the information from Table 5.1.

x = ... [1]

(ii) The mass spectrum of **W** also shows peaks at *m*/*e* = 29 and *m*/*e* = 59.

Suggest the molecular formulae of these fragments.

m/*e* = 29 .....

m/*e* = 59 .....

[2]

3 **(e)** Compound **F** reacts with reagent **G** to form compound **H**.

The infrared spectrum of **H** is shown in Fig. 4.3.

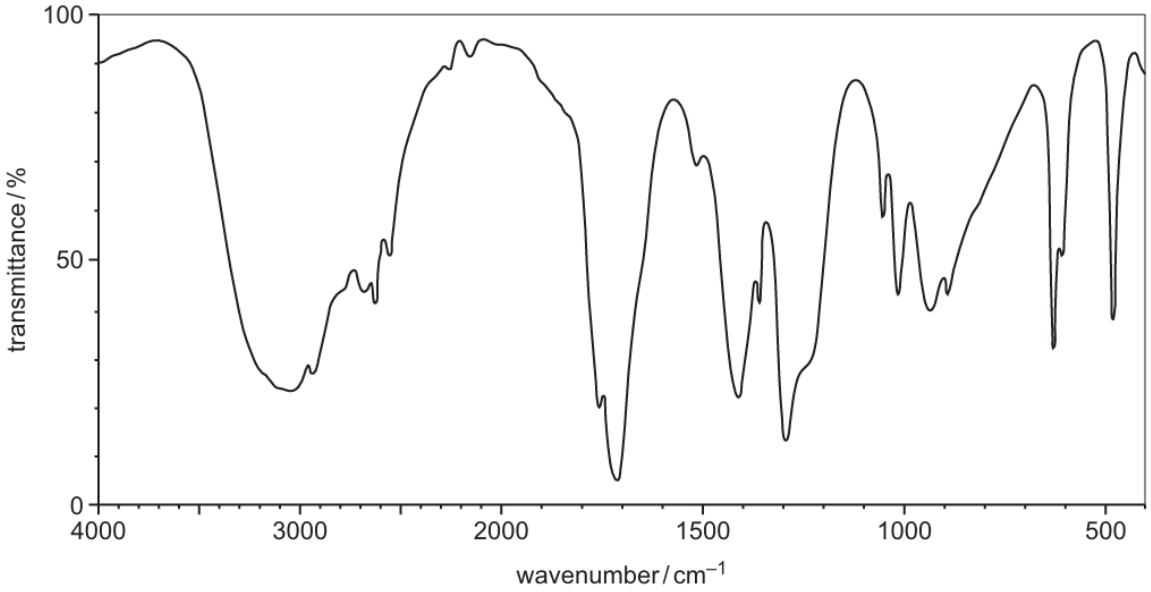


Fig. 4.3

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 3200–3600

H also shows a molecular ion peak at *m*/*e* = 60 in its mass spectrum.

(i) Use the information in **(e)**, Fig. 4.3 and Table 4.2 to deduce the structure of **H**. Explain your answer fully.

H

.....

.....

.....

[3]

(ii) Suggest the role of reagent **G**.

.....

[1]

4 Chlorine is a very reactive element.

(f) **X** is a product of the substitution reaction that occurs when $CHCl F_2$ reacts with Br_2.

There is only one naturally occurring isotope of fluorine, ^{19}F.

The mass spectrum of **X** shows molecular ion peaks at *m*/*e* = 164, 166 and 168.

Complete Table 3.3 to show **all** the molecular ions responsible for each peak.

Table 3.3

m/*e*	formulae of molecular ions
164	
166	
168	$(CF_2{}^{37}Cl^{81}Br)^+$

[2]

5 Compounds **C** and **D** are alkenes with the same molecular formula, C_5H_{10}.

Fig. 4.1

(b) The mass spectrum of **C** shows a molecular ion peak at *m*/*e* = 70. This peak has a relative intensity of 48.7.

The relative intensity of the [M+1] peak is 2.7.

Show that this information is consistent with the molecular formula of **C**.

[2]

6 Compound **V** is a liquid.

V contains 77.2% carbon, 11.4% hydrogen and 11.4% oxygen by mass.

V has a relative molecular mass of 280.

(d) Fig. 5.1 shows the mass spectrum of ketone **Z**, $C_5H_{10}O$.

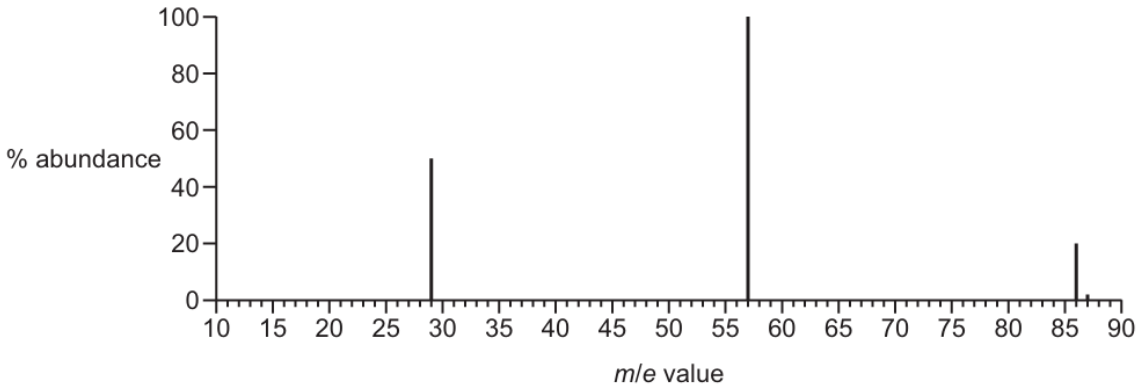


Fig. 5.1

Use the information in Fig. 5.1 to suggest the formulae of the fragments with *m/e* peaks at 29 and 57. Deduce the identity of **Z**.

m/e = 29 .....

m/e = 57 .....

identity of **Z** .....

[3]

7 **Z** is a molecule which contains the elements carbon, hydrogen and oxygen only.

Z contains only alkene and carboxyl functional groups.

(c) Fig. 6.1 shows the mass spectrum of **Z**.

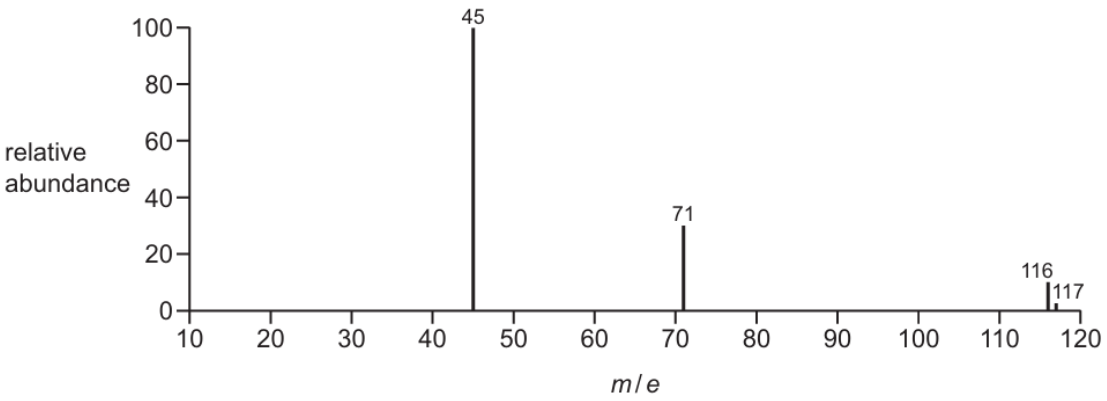


Fig. 6.1

(i) Deduce the molecular formula of **Z**. Explain your answer by referring to the molecular ion peak in Fig. 6.1 and the empirical formula of **Z**.

[1]

(ii) Use Fig. 6.1 to suggest the formulae of the fragments with *m*/*e* peaks at 45 and at 71.

m/*e* 45 .....

m/*e* 71 .....

[2]

(iii) Suggest the structure of **Z** using relevant information from Table 6.1, **(b)** and **(c)**.

[1]

8 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.

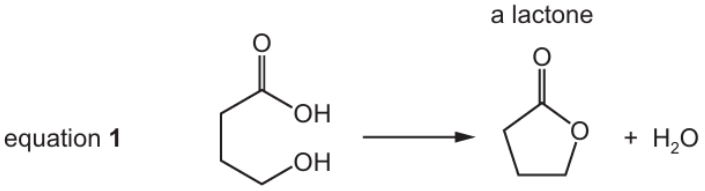


Fig. 5.1 shows the synthesis of lactone **P** from compound **M**.

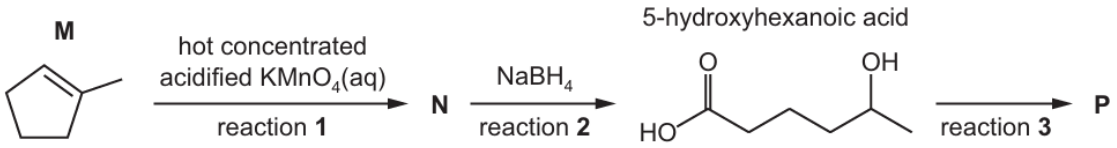


Fig. 5.1

(c) Unknown lactone **Q** is analysed using mass spectrometry.
Table 5.2 shows information from the mass spectrum.

Table 5.2

peak	*m/e*	abundance
M+	72	95.5
M+1	73	3.15

Use these data to deduce the structure of **Q**.
Show your working.

Q

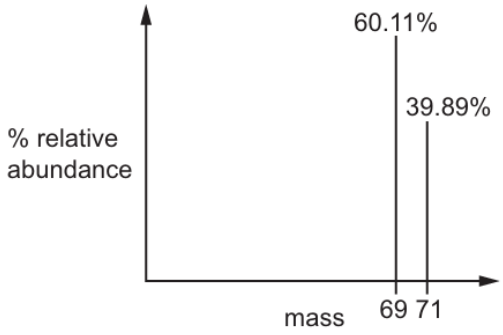
.....

.....

[2]

9 Gallium is an element in Group 13.

A sample of gallium is analysed using a mass spectrometer. The mass spectrum produced is shown.



(b) Calculate the relative atomic mass of gallium in this sample. Give your answer to 4 significant figures.

Show your working.

relative atomic mass = ... [2]