22.2 MASS SPECTROMETRY- WORKSHEET

Introduction

1. Which of the following corresponds to the **base peak** in a mass spectrum?
   A The peak corresponding to the ion with the lowest m/e.
   B The peak corresponding to the molecular ion.
   C The peak corresponding to any ion formed by the fragmentation of the molecule.
   D The peak corresponding to the most abundant ion.

Determination of A_r from mass spectra

2. The mass spectrum of a sample of lithium shows that it contains two isotopes, ^{6}Li and ^{7}Li.
   The isotopic abundances are shown in the table.

isotope	isotopic abundance
^{6}Li	7.42%
^{7}Li	92.58%

   What is the relative atomic mass of this sample of lithium, given to three significant figures?

   A 6.07 **B** 6.50 **C** 6.90 **D** 6.93

3. A sample of sulfur consists mostly of ^{32}S. It also contains 4.2% ^{34}S and 2.8% ^{36}S. No other isotopes of sulfur are present.
   What is the relative atomic mass, A_r, of **this** sample of sulfur?

   A 32.1 **B** 32.2 **C** 34.0 **D** 34.3

4. The element sulfur produces a mass spectrum with the following peaks.

m / e value of peak	Relative abundance
32	95.02
33	0.76
34	4.20
36	0.02

   Which relative atomic mass of sulfur can be calculated from these data, given to four significant figures?

   A 32.07 B 32.08 C 32.09 D 32.10

1. A sample of magnesium contains three isotopes, ^{25}Mg, ^{26}Mg and **X**.
The percentage abundance of the three isotopes is shown in Table 1.1.

isotope of Mg	mass/a.m.u.	percentage abundance/%
X		78.99
^{25}Mg	24.99	10.00
^{26}Mg	25.98	11.01

Calculate the mass of **X**. Use data from above table and A_r (magnesium) = 24.31 in your calculation.
Show your working. [2]

5. A sample of magnesium contains the isotopes ^{24}Mg, ^{25}Mg and ^{26}Mg only.
The percentage abundance of ^{25}Mg and ^{26}Mg is the same.
The relative atomic mass of magnesium in the sample is 24.3.
What is the percentage abundance of ^{24}Mg?

A 10% B 20% C 60% D 80%

2. The relative atomic mass of gallium, $\mathbf{A}_r$, is 69.723.
The relative isotopic masses of ^{69}Ga and ^{71}Ga are:
^{69}Ga, 68.926; ^{71}Ga, 70.925.
Use this information to calculate the percentage abundance of ^{69}Ga in elemental gallium.
Show your working.
Assume that the element contains only the $_{69}Ga$ and $_{71}Ga$ isotopes.
Give your answer to four significant figures. [2]

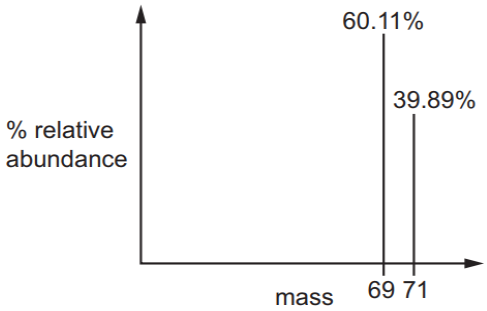
3. Table 1.2 shows the relative abundances of isotopes in a sample of an alloy containing rhodium and iridium only.

isotope	relative isotopic mass	relative abundance in alloy
$^{103}_{45}Rh$	102.91	50.00
$^{191}_{77}Ir$	190.96	15.18
$^{193}_{77}Ir$	192.96	34.82

Use Table 1.2 to calculate the relative atomic mass, Ar, of iridium in the alloy.
Give your answer to two decimal places.

relative atomic mass of iridium = ... [2]

4. Gallium is an element in Group 13.
A sample of gallium is analysed using a mass spectrometer. The mass spectrum produced is shown.



Calculate the relative atomic mass of gallium in this sample. Give your answer to 4 significant figures.
Show your working. [2]

5. A sample of sulfur contains only two isotopes, $_{32}S$ and $_{34}S$. The relative atomic mass of this sample is 32.09.

isotope	isotopic mass
$_{32}S$	32.0
$_{34}S$	34.0

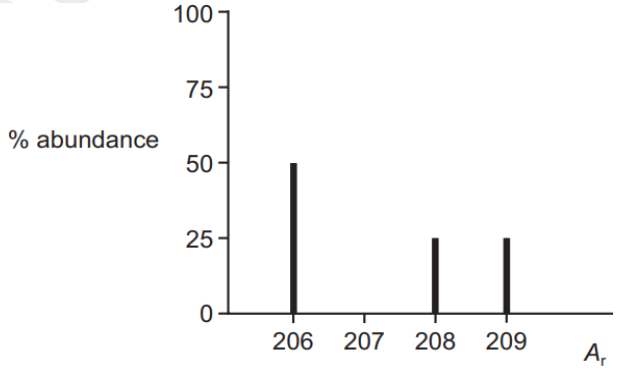
Calculate the percentage abundance of the isotopes present in this sample. [3]

6. Silicon is found in many compounds in the Earth's crust. Silicon has only three naturally occurring isotopes, ^{28}Si, ^{29}Si and ^{30}Si.
The table shows data for ^{28}Si, ^{29}Si and ^{30}Si.

	^{28}Si	^{29}Si	^{30}Si
relative isotopic mass	28.0	29.0	30.0

A sample of silicon contains 92.2% $_{28}Si$. The total percentage abundance of $_{29}Si$ and $_{30}Si$ in the sample is 7.8%.
The relative atomic mass, A_r, of silicon in the sample is 28.09.
Calculate the percentage abundance of $_{30}Si$.
Give your answer to **one** decimal place. [3]

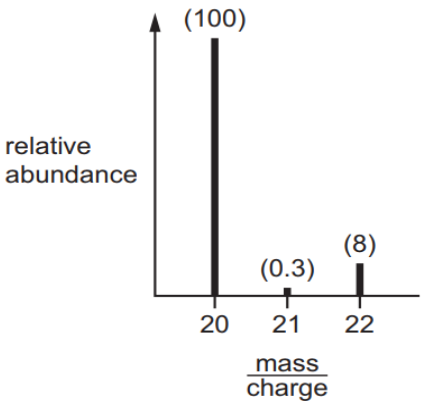
6. The diagram shows the relative abundance of different isotopes of lead in a sample of lead ore.
The abundance of 208 is half that of 206. The abundances of 208 and 209 are equal.



What is the relative atomic mass of the lead in the sample?

A 207.00 **B** 207.25 **C** 207.50 **D** 207.67

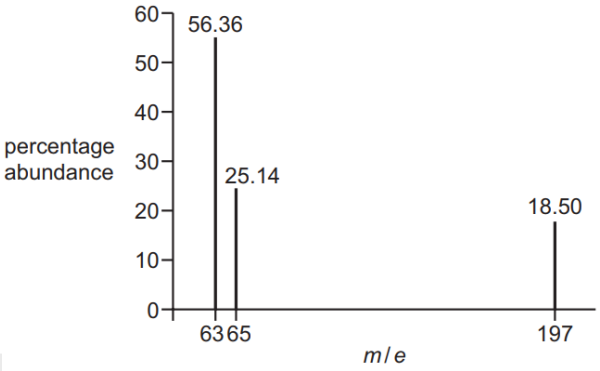
7. The mass spectrum of a sample of neon is shown. The relative abundance of each peak is written in brackets above it.



What is the relative atomic mass, Ar, of this sample of neon?

A 20.15 **B** 20.20 **C** 21.00 **D** 21.82

8. The mass spectrum of an alloy of copper and gold is shown



Which expression can be used to calculate the relative atomic mass, Ar, of copper present in this sample?

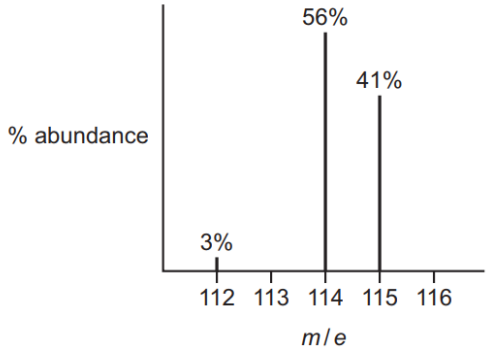
A $\dfrac{(56.36 \times 63)+(25.14 \times 65)}{(56.36+25.14+18.50)}$

B $\dfrac{(56.36 \times 63)+(25.14 \times 65)+(18.50 \times 197)}{(56.36+25.14+18.50)}$

C $\dfrac{(56.36 \times 63)+(25.14 \times 65)}{(56.36+25.14)}$

D $\dfrac{(56.36 \times 63)+(25.14 \times 65)}{(63+65)}$

9. A sample of element X is analysed using mass spectrometry. The mass spectrum obtained is shown.



What is the relative atomic mass of this sample of element X?

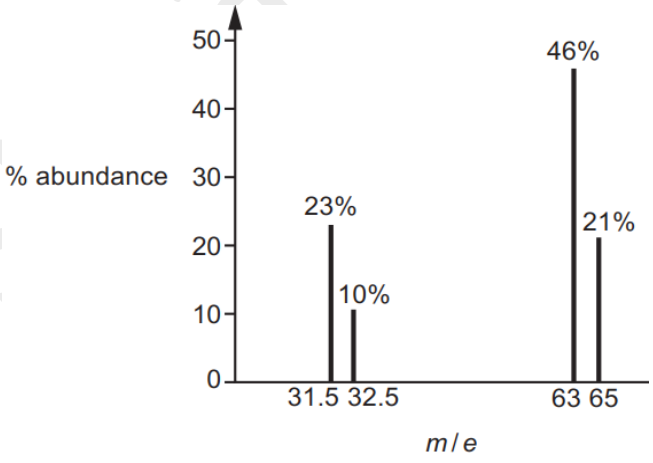
A 113.7 **B** 114.0 **C** 114.2 **D** 114.4

7. The relative isotopic masses and natural abundances of the two isotopes in a sample of copper are shown in the following table.

isotope	relative isotopic mass	% abundance
^{63}Cu	62.930	69.15
^{65}Cu	64.928	30.85

(i) Calculate the relative atomic mass, A_r, of copper in this sample using the data in the above table. Show your working. [1]

(ii) The mass spectrum of a sample of pure copper is shown in the following figure.



Identify the ion with an abundance of 23% in the sample. [1]

8. A sample of iron is analysed using a mass spectrometer. The mass spectrum shows three isotopes of iron are present in the sample.
Fig. 2.1 shows the mass spectrum of the sample of iron.

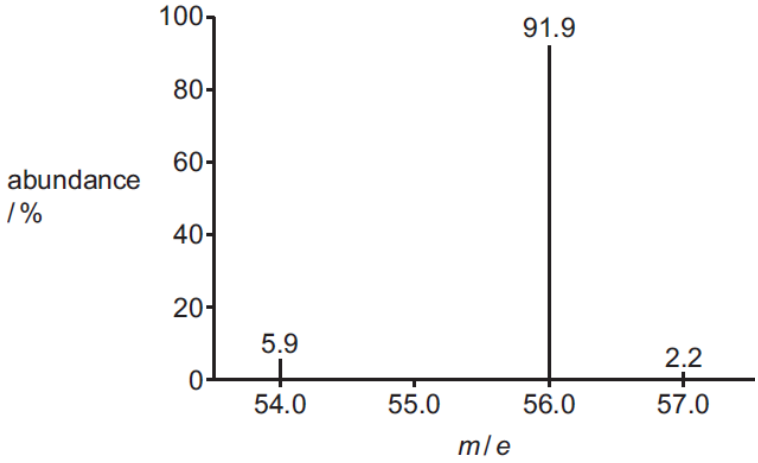


Fig. 2.1

Use Fig. 2.1 to calculate the relative atomic mass, Ar, of iron to one decimal place.
Show your working.

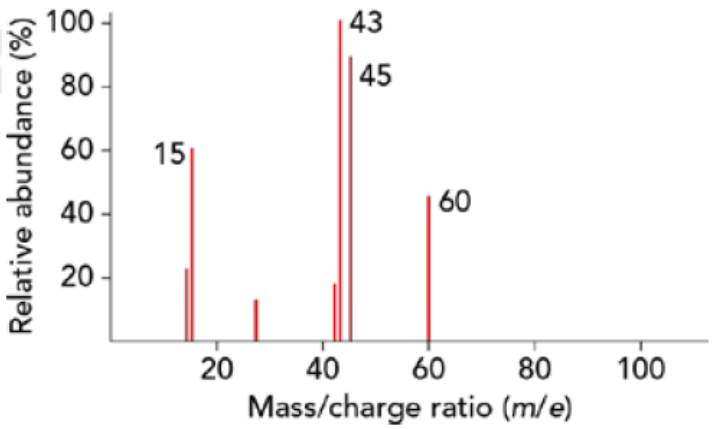
Ar of iron = ... [2]

10. A sample of gallium contains two isotopes only.
In every 10 atoms in the sample, there are 6 that have 38 neutrons and 4 that have 40 neutrons.
What is the relative atomic mass, *A*r, of the gallium in the sample?

A 69.7 B 69.8 C 70.0 D 70.2

Identification of an organic compound using mass spectrometry

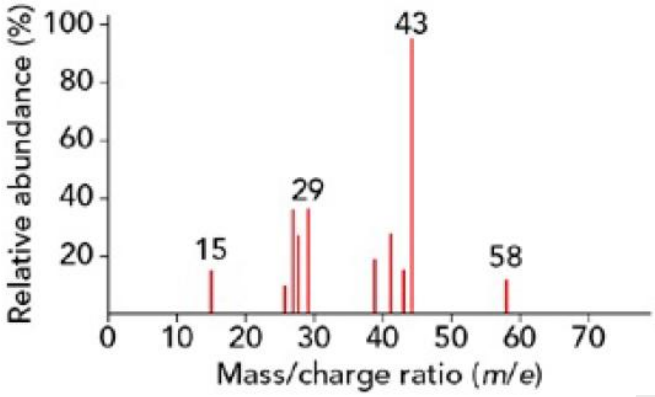
1. Look at the mass spectrum of ethanoic acid:



Identify the fragments with mass-to-charge ratios of:

a 15 B 43 C 45 D 60

2. The mass spectrum of an organic compound with the structure $CH_3CH_2CH_2CH_3$ is shown.



Identify the fragments with mass/charge ratios of

15, 29, 43, 58

11. Three organic compounds are listed.
1 ethanal
2 propan-1-ol
3 propan-2-ol
Which compounds will have a mass spectrum that contains a fragment peak at *m* / *e* = 43?

A 1 only **B** 1 and 2 only **C** 2 and 3 only **D** 1, 2 and 3

12. Which alcohol is **not likely** to have fragmentation ion at m/e = 43 in its mass spectrum?

A $(CH_3)_2CHCH_2OH$

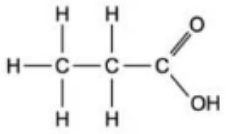
B $CH_3CHOHCH_2CH_2CH_3$

C $CH_3CH_2CH_2CH_2OH$

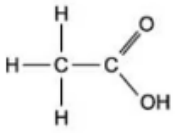
D $CH_3CH_2CHOHCH_3$

13. Which of the following molecule is **not likely** to have fragment ion at m/e = 43 in its mass spectrum?

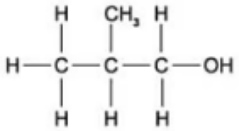
A.



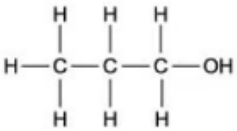
B.



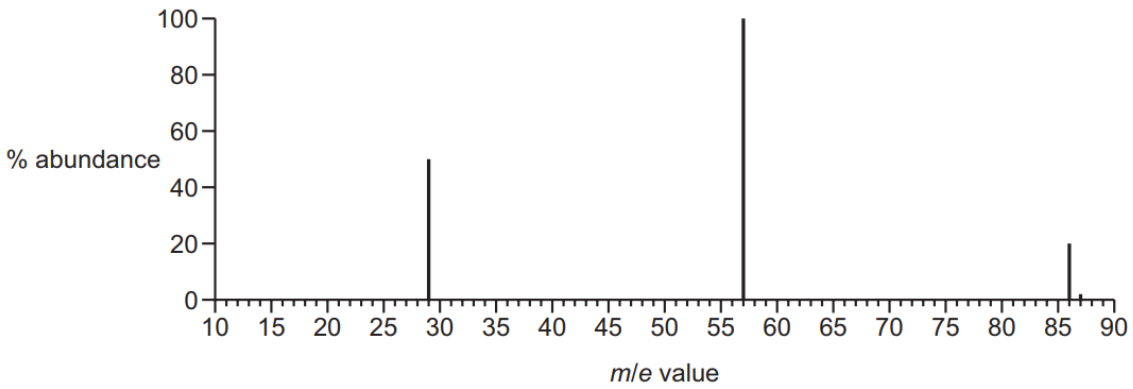
C.



D.



3. Figure below shows the mass spectrum of ketone **Z**, $C_5H_{10}O$.



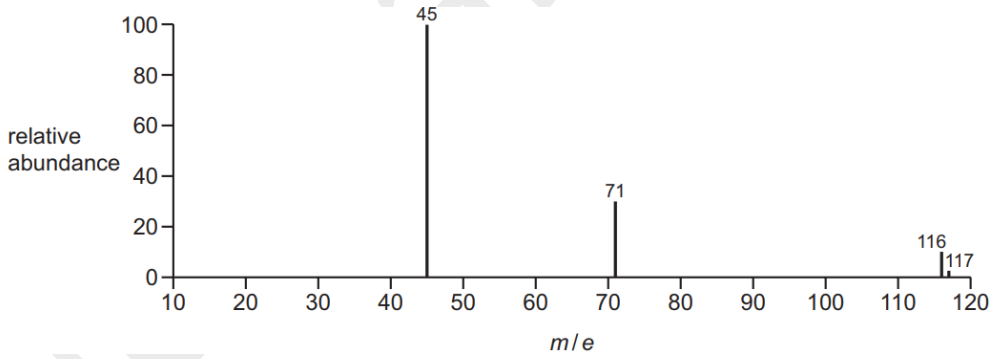
Use the information in Fig. 5.1 to suggest the formulae of the fragments with **m/e** peaks at 29 and 57. Deduce the identity of Z. [3]

4. **Z** is a molecule which contains the elements carbon, hydrogen and oxygen only.
Z contains only alkene and carboxyl functional groups.
(a) Table 6.2 shows the percentage by mass of each element present in **Z**.

element	percentage by mass/%
carbon	41.38
hydrogen	3.45
oxygen	55.17

(i) Using the data in Table 6.2, demonstrate that the empirical formula of **Z** is CHO.
Show your working. [1]

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



(ii) 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]

(iii) Use Fig. 6.1 to suggest the formulae of the fragments with **m** /**e** peaks at 45 and 71. [2]

(iv) Suggest the structure of **Z** using relevant information from Table 6.1, **(b)** and **(c)**. [1]

5. Look at Figure 3.10, which shows the mass spectrum of ethanol, C_2H_5OH. A structural isomer of ethanol is methoxymethane, an ether with the formula CH_3OCH_3.

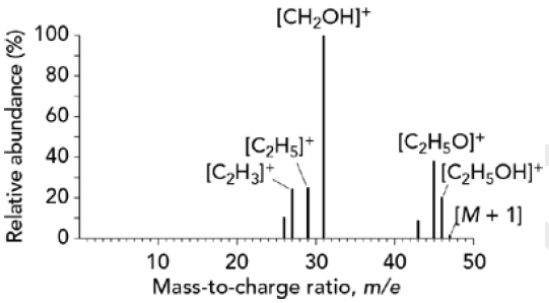


Fig: 3.10 mass spectrum of ethanol

a. Predict the mass-to-charge ratio of a fragment that would appear on the mass spectrum of methoxymethane but does not appear on ethanol's mass spectrum.

b. Give the formula of the ion responsible for the peak in your answer to part a.

Deduce the number of carbon atoms, *n*, in a compound using the M +1 peak

and the formula

n =100 × abundance of M+1 ion/(1.1 × abundance of M^+ ion)

6. A hydrocarbon has a molecular ion peak at a mass-to-charge ratio of 84 (relative abundance of 62.0%) and an [*M*+1] peak with a relative abundance of 4.1%.
How many carbon atoms are in the hydrocarbon?

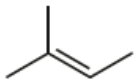
7. An organic compound, Z, has a molecular ion peak, *M*, with a relative abundance of 36.4% and an [*M* + 1] peak with a relative abundance of 4.8 %. Deduce the number of carbon atoms this compound contains.

14. In the mass spectrum of a compound, Z, the relative abundances of the M and M+1 peaks are in the ratio 13: 1.
What is compound Z?

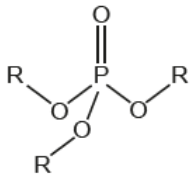
A butyl butanoate **B** hexan-3-one **C** 2,2,3-trimethylhexane **D** 3,3-dimethylpentan-1-ol

8. 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]

C



9. H_3PO_4 also reacts with alcohols to form organophosphates.
Organophosphates are compounds similar to esters. They have the general structure shown in figure below.



R = alkyl group

Compound **T** is a simple organophosphate.
The mass spectrum of **T** shows a molecular ion peak at $m / e = 182$. This peak has a relative intensity of 12.7.
The relative intensity of the M +1 peak is 0.84.
Deduce the number of carbon atoms in **T**.
Hence suggest the molecular formula of **T**.
Assume that phosphorus and oxygen exist as single isotopes.
Show your working.

number of carbon atoms in **T** = ...

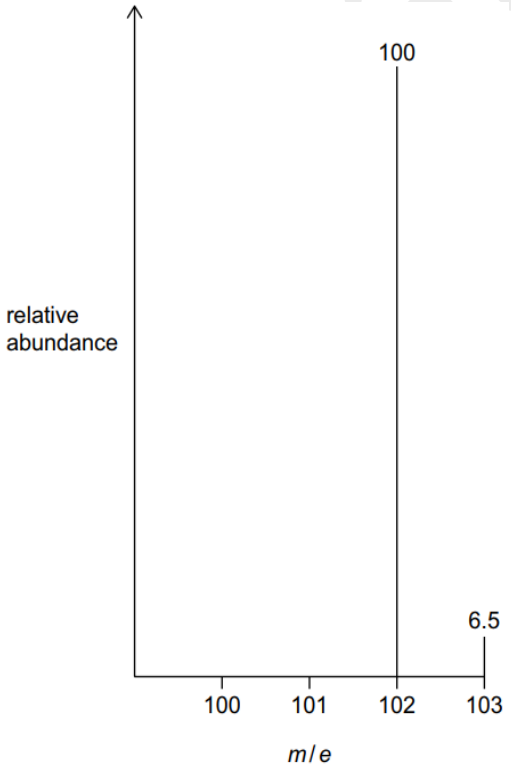
molecular formula of **T** = ... [3]

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

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. [2]

19. Compound **X** contains atoms of carbon, hydrogen and oxygen only.
The mass spectrum of **X** is recorded. Information about the two peaks with m/e greater than 100 is shown in Fig. 5.1.



(a) A molecule of **X** contains 6 carbon atoms.
Demonstrate that this is correct using information from the above figure. Show your working. [2]

(b) Suggest the molecular formula of **X** using information in the above figure. [1]

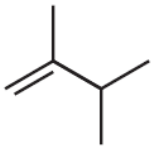
(c) Suggest the molecular formula of the fragment of **X** at m / e = 31. [1]

15. Oxygen has three stable isotopes, ^{16}O, ^{17}O and ^{18}O. All three isotopes are present in a sample of oxygen gas, O_2, which was analysed using a mass spectrometer.
How many peaks associated with the O_2^+ ion would be expected?

A 3 **B** 5 **C** 6 **D** 9

20. Under different conditions, two molecules of propene can combine to form compounds X and Y.

X



Y

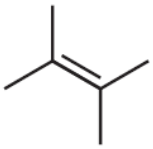


Fig. 4.2 shows the mass spectrum of either compound X or compound Y.

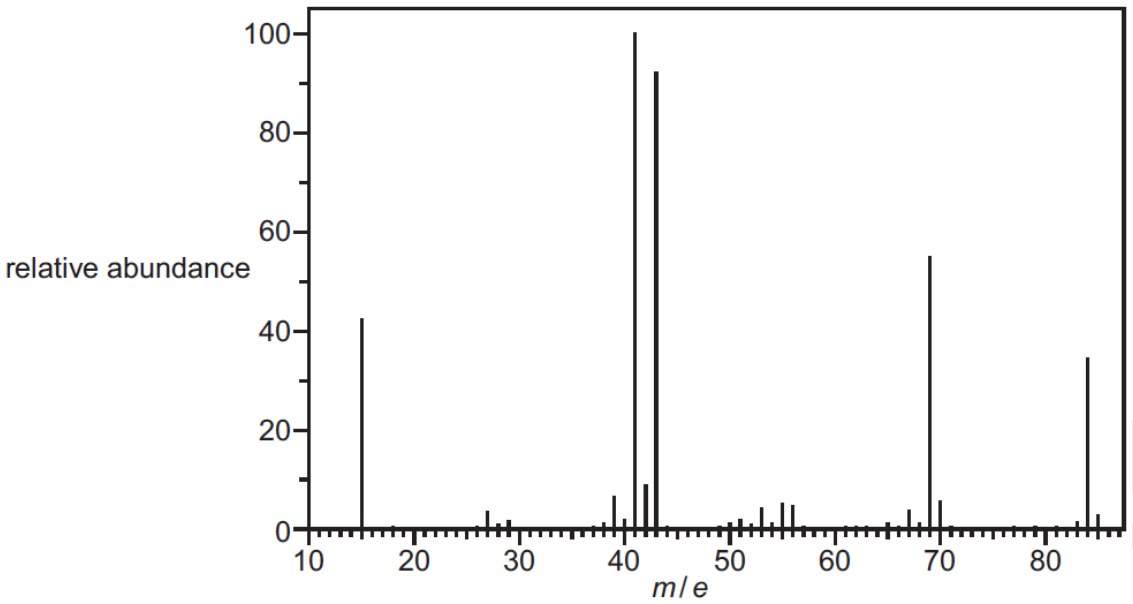


Fig. 4.2

Identify which of X and Y gives this mass spectrum.
Give one reason for your answer, referring to the fragmentation pattern.

.....

.....

..... [1]

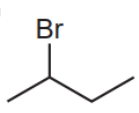
(iii) The molecular ion peak in the spectrum in Fig. 4.2 has relative abundance 34.7.
Calculate the relative abundance of the [M+1]+ peak in this spectrum.

relative abundance of [M+1]+ peak = ... [1]

Deduce the presence of bromine and chlorine atoms in a compound using the M +2 peak

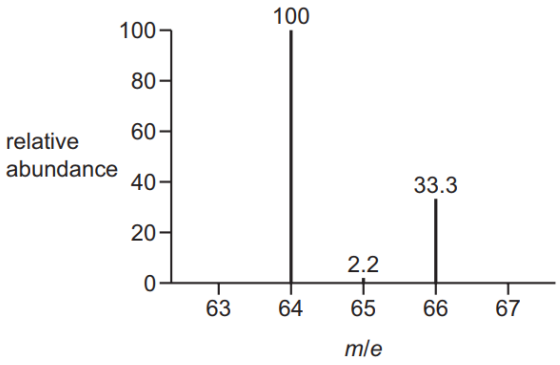
21. In the mass spectrum of **D**, the relative abundance of the molecular ion peak is 3.4.

D



Predict the relative abundance of the M+2 peak for **D**.
Explain your answer. [1]

22. **Z** contains three types of atom: carbon, hydrogen and a halogen. The mass spectrum of **Z** is recorded.
Fig. 5.1 shows a section of the mass spectrum at **m**/**e** greater than 63.
The fragment at **m**/**e** = 64 is the molecular ion peak.



(i) Deduce the number of carbon atoms present in a molecule of **Z** using above figure.
Show your working. [1]

(ii) Deduce which halogen is present in **Z** using Fig. 5.1. Explain your answer. [1]

(iii) There are also peaks at **m**/**e** = 29 and **m**/**e** = 49.
Suggest the formulae of these fragments.
Deduce the name of Z. [3]

16. The mass spectrum of compound X has M, M+1 and M+2 peaks. Other peaks are also present.
Peak M is the molecular ion peak, M+. Peak M has a relative abundance fifteen times that of peak M+1.
Peaks M and M+2 are of equal height.
What could be compound X?

A 1-chloro-2,2-dimethylpentane
B 2-chloro-3-methylpentane
C 2-bromo-2-methylhexane
D 3-bromo-2,2-dimethylbutane

17. There are two naturally occuring isotopes of bromine. One isotope has 44 neutrons. The other isotope has 46 neutrons.

Ignoring fragments, how many peaks are there in the mass spectrum of tribromomethane, $^{12}C^{1}HBr_3$?

A 2 B 3 C 4 D 6

23. 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]

(iii) 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**.

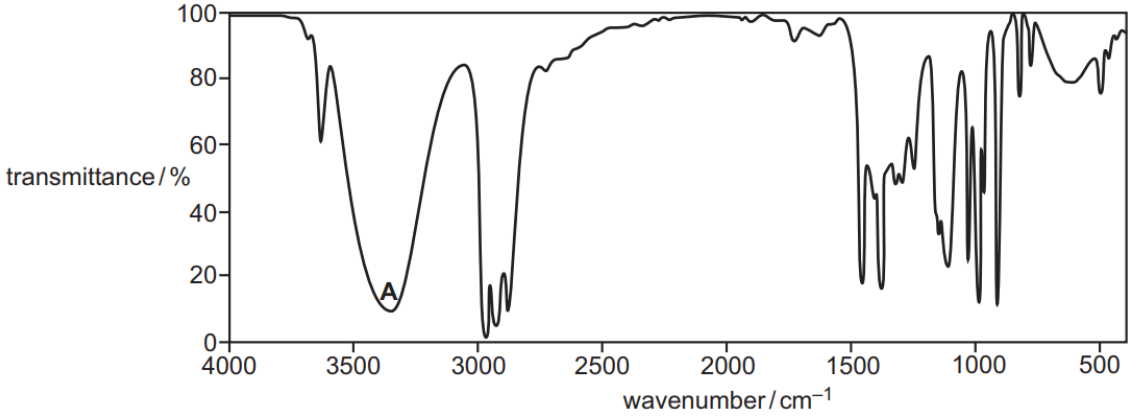
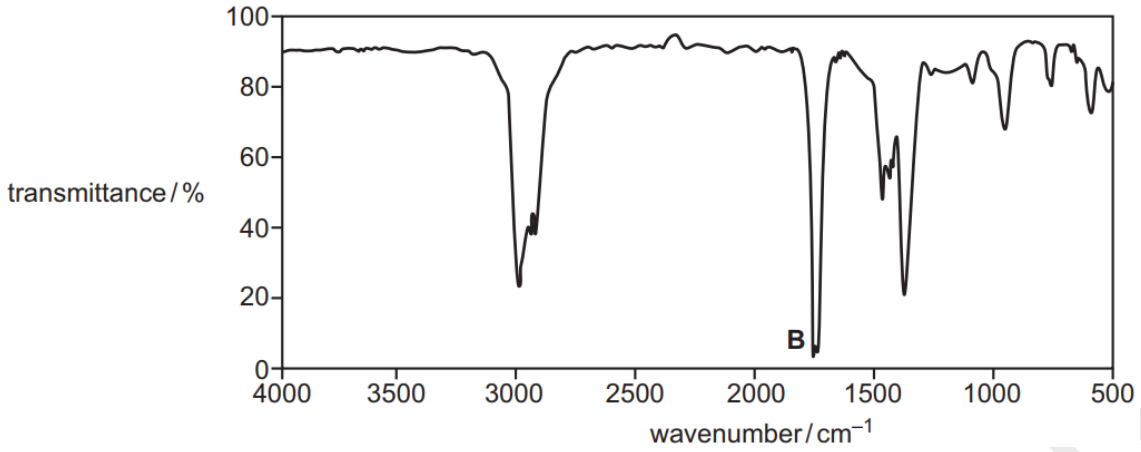


Fig. 5.2 shows the infrared spectrum of **X**.



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

absorption	bond	functional group containing the bond
A		
B		

(iv) Use the information in **(a)** and **(b)(i)** to draw the structure of **X** in the box in Fig. 5.3.

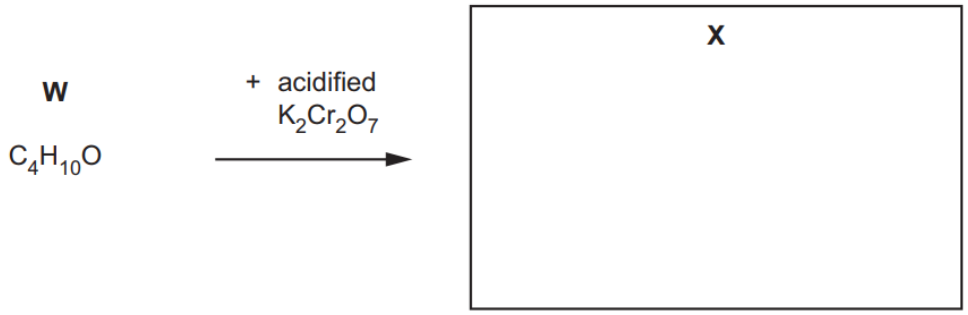


Fig. 5.3

[1]

b) **Y** is a structural isomer of **W**.
Both **W** and **Y** produce colourless bubbles when sodium is added to them.
Y does **not** react when heated with acidified $K_2Cr_2O_7$.
Y does **not** react when warmed with alkaline $I_2(aq)$.
(i) Name the functional group present in **Y**.

.....
... [1]

(ii) Complete the equation to describe the reaction of **W** or **Y** with sodium.

.....$C_4H_{10}O$ + ...Na
..... [1]

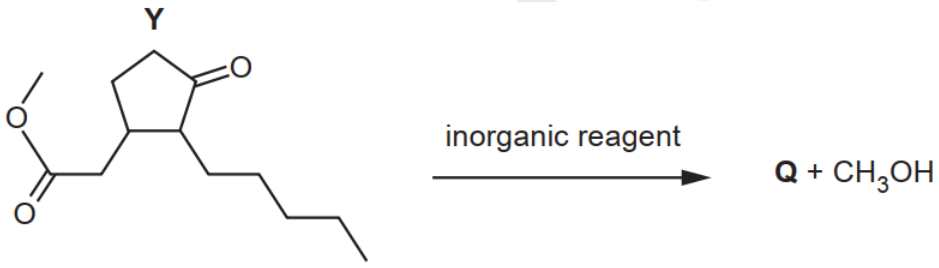
(iii) Draw the structure of **Y**. [1]

24. X is a product of the substitution reaction that occurs when $CHClF_2$ 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 the following table to show **all** the molecular ions responsible for each peak. [2]

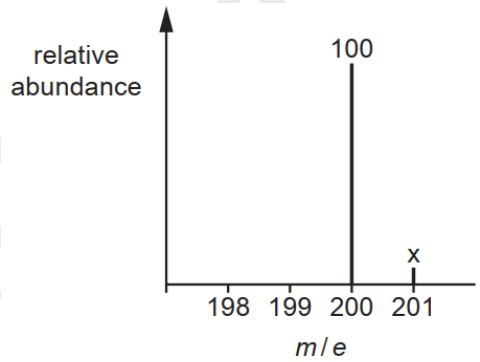
m/e	formulae of molecular ions
164	
166	
168	$(CF_2{}^{37}Cl\ {}^{81}Br)^+$

The mass spectrum of chlorobutane shows an [M + 2] peak beyond the M_r peak. Explain why there is an [M + 2] peak.
The relative height of the [M + 2] peak in organic compound T is the same as that of the M_r peak. Explain how this shows that the compound contains one atom of bromine and not one atom of chlorine.

25. 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.



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



(i) Calculate the relative abundance, x, of the peak at **m/e** = 201.
Show your working.

[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**. **[1]**

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

(iii) Under certain conditions, 0.0020mol of **Q** reacts with an excess of sodium to produce a total of 44.8cm3 of gas at s.t.p.
Calculate the number of hydroxyl groups present in a molecule of **Q**.
Show your working.

(iv) Use Table 6.2 to describe and explain **two** differences between the infrared spectrum of **Y** and **Q** in the region above 1500cm^{-1}. [2]

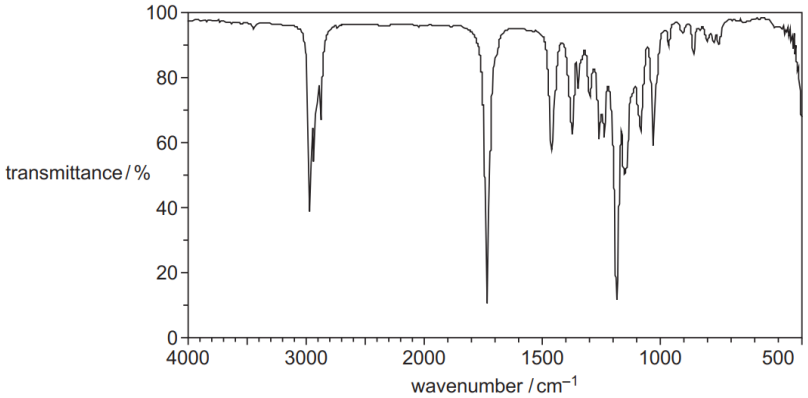
26. Compounds **S** and **T** react to form organic compound **U**, which has a single functional group.

Table 4.2 shows some data from the mass spectrum of **U**.

peak	relative abundance
M+	7.2
[M+1]+	0.55

(i) Use the data from Table 4.2 to show that **U** contains 7 carbon atoms.
Show your working.

(ii) Fig. 4.2 shows the infrared spectrum of **U**.



Use Fig. 4.2 to identify the functional group present in **U**.
Explain your answer fully.

functional group .....

explanation.....

.....

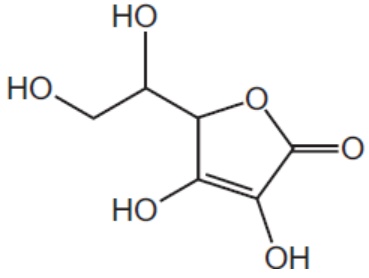
..... [2]

T also has a single functional group.
Use the information in **(c)(i)** and your answer to **(c)(ii)** to identify **T** and **U**.
Draw the structures of **T** and **U** in the boxes. [2]

c) A scientist chooses either infrared spectroscopy or mass spectrometry to find a particular piece of information.
In which row has the **best** choice been made?

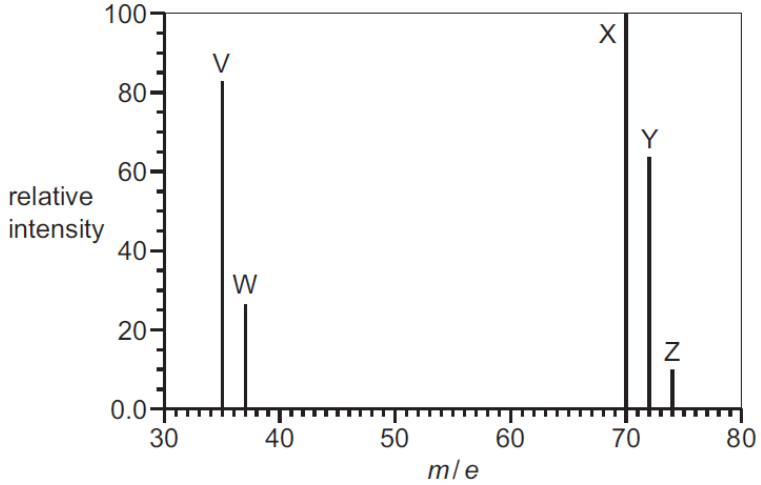
	target information	analytic method used
A	identities of functional groups in an organic compound	infrared spectroscopy
B	identities of functional groups in an organic compound	mass spectrometry
C	values of successive ionisation energies of Na	infrared spectroscopy
D	values of successive ionisation energies of Na	mass spectrometry

18. Vitamin C has the structure shown.



The mass spectrum of vitamin C has a molecular ion peak with an m/e value of 176 and a relative abundance of 7.0%.
What is the abundance of the M +1 peak?
A 0.462% B 0.539% C 0.616% D 0.693%

19. The diagram shows the mass spectrum of a sample of chlorine. Peaks V, W, X, Y and Z are labelled.



Which statements about this spectrum are correct?

1 The relative atomic mass of chlorine can be calculated from the abundances and m / e values of 2 of the 5 peaks.

2 37.0 g of the species responsible for peak Z contains 3.011 □ 1023 molecules.

3 The relative molecular mass of chlorine can be calculated from the abundances and m / e values of peaks X, Y and Z.

A 1, 2 and 3 B 1 and 2 only C 1 and 3 only D 2 and 3 only

27. CH_3CH_2COOH reacts with an unsaturated alcohol R to form unsaturated ester S.

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

..... [1]

The infrared spectrum of S is shown in Fig. 4.2.

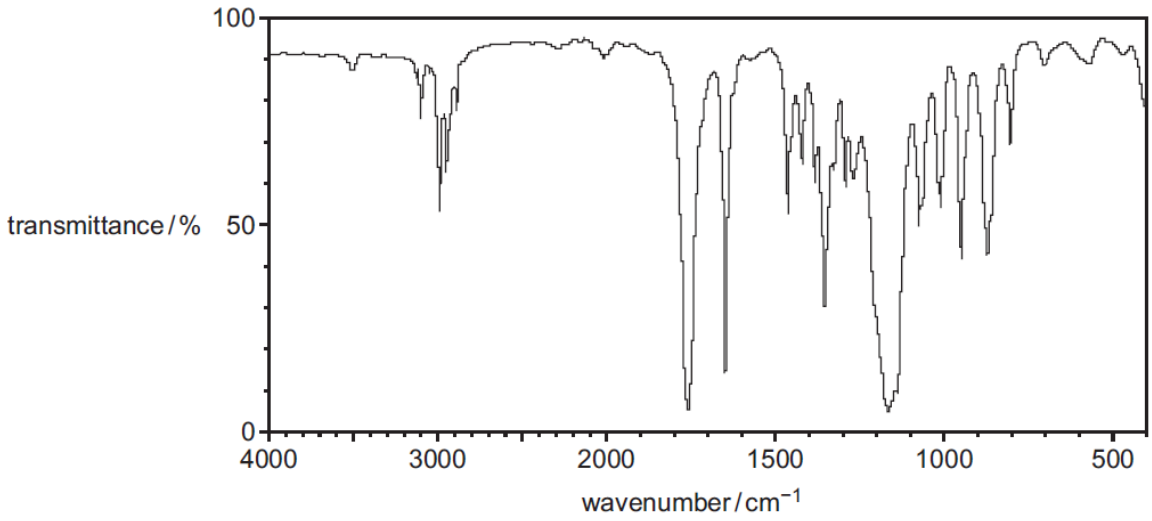


Fig. 4.2

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.

absorption	1	2	3
bond responsible			

(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]

28. Q reacts with HBr(g) to produce two structural isomers, R and S, as shown in Fig. 4.2.

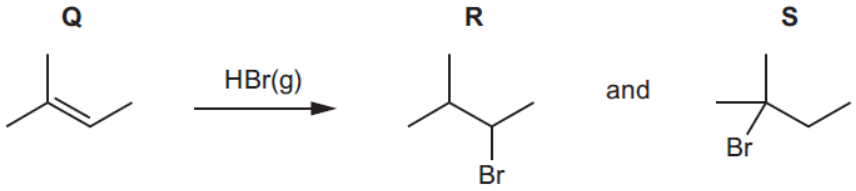


Fig. 4.2

The mass spectrum of R shows peaks at m / e = 150 and m / e = 152.
Suggest structures for the ions responsible for these peaks. [2]

peak at *m/e* = 150	peak at *m/e* = 152

***..... ***