Mass Spectrometry

Question Paper 1

Level	International A Level
Subject	Chemistry
Exam Board	CIE
Topic	Analytical techniques
Sub-Topic	Mass Spectrometry
Paper Type	Theory
Booklet	Question Paper 1

Time Allowed: **75 minutes**

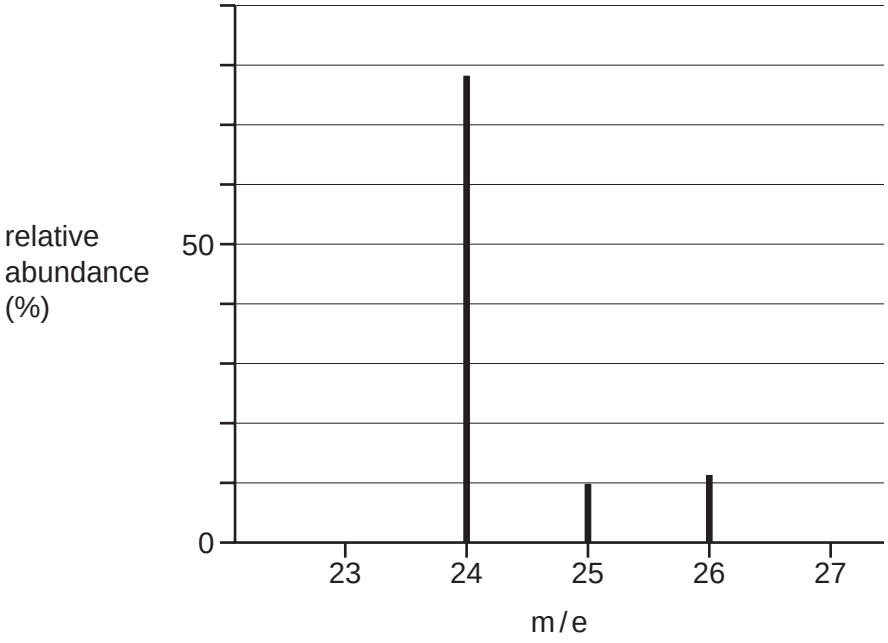
Score: **/62**

Percentage: **/100**

Grade Boundaries:

A*	A	B	C	D	E	U
>85%	777.5%	70%	62.5%	57.5%	45%	<45%

1 **(a)** The mass spectrum of the element magnesium is shown below.



(i) From the mass spectrum, complete the table with the relative abundances of the three isotopes.

isotope	relative abundance
^{24}Mg	
^{25}Mg	
^{26}Mg	

[1]

(ii) Use your values in **(i)** to calculate the relative atomic mass, A_r, of magnesium to **two** decimal places.

A_r (Mg) = ... [1]

(b) (i) Describe and explain the trend in the thermal stabilities of the nitrates of the Group II elements down the group.

.....

.....

.....

.....

..... [3]

When lithium nitrate, $LiNO_3$, is heated, it readily decomposes giving off a brown gas. This reaction is similar to that which occurs when magnesium nitrate is heated, but it does not occur with other Group I nitrates.

(ii) Suggest an equation for the action of heat on $LiNO_3$.

..... [1]

(iii) Suggest why the Group I nitrates other than $LiNO_3$ do **not** decompose in this way when heated.

.....

..... [1]

[Total: 7]

2 **(a)** NMR spectroscopy and X-ray crystallography can both be used to examine the structure of organic compounds.

NMR is very useful at examining hydrogen atoms in compounds, but hydrogen atoms are invisible to X-rays.

(i) Explain why NMR spectroscopy can detect hydrogen atoms in molecules.

.....

..... [1]

(ii) Explain why hydrogen atoms are invisible to X-rays.

.....

.....

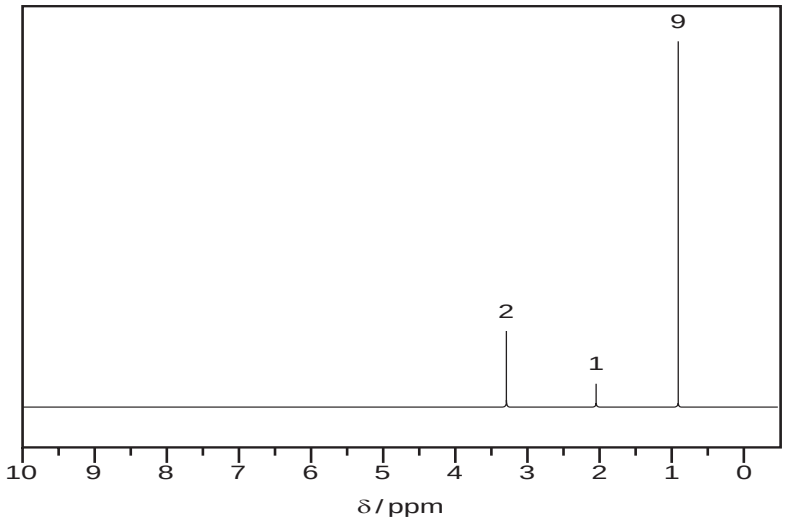
(iii) The molecular formula of the amino acid cysteine is $C_3H_7O_2NS$.

Explain which of the atoms present would show the greatest absorption on exposure to X-rays. [1]

.....

..... [1]

(b) The NMR spectrum below was obtained from an organic liquid, **P**, which contains five carbon atoms per molecule.



(i) How many protons are present in one molecule of **P**? Explain your answer.

number of protons .....

.....

..... [1]

(ii) When a little D_2O is added to **P**, the absorption at δ2.0 disappears.

Explain what this tells you about the group responsible for this absorption and why.

.....

.....

..... [2]

(iii) What does the absorption at δ0.9 tell you about the adjacent carbon atom?

.....

..... [1]

(iv) What group(s) is/are responsible for the absorption at δ0.9?

..... [1]

(v) Suggest a structure for **P**.

[1]

(c) When an isomer of **P** is heated with concentrated H_2SO_4 it forms a new compound, **Q**. This new compound **Q** reacts with bromine to give a dibromide, **R**.

(i) A mass spectrum was obtained of **R**. The ratio of the heights of the M : M+1 peaks was 9.3 : 0.5.

Show that there are five carbon atoms present in one molecule of **R**.

[1]

(ii) Predict the ratio of the heights of the M : M+2 : M+4 peaks as a result of the two bromine atoms in the dibromide **R**. Show your working.

ratio ..... [1]

(iii) What is the molecular formula of **R**?

..... [1]

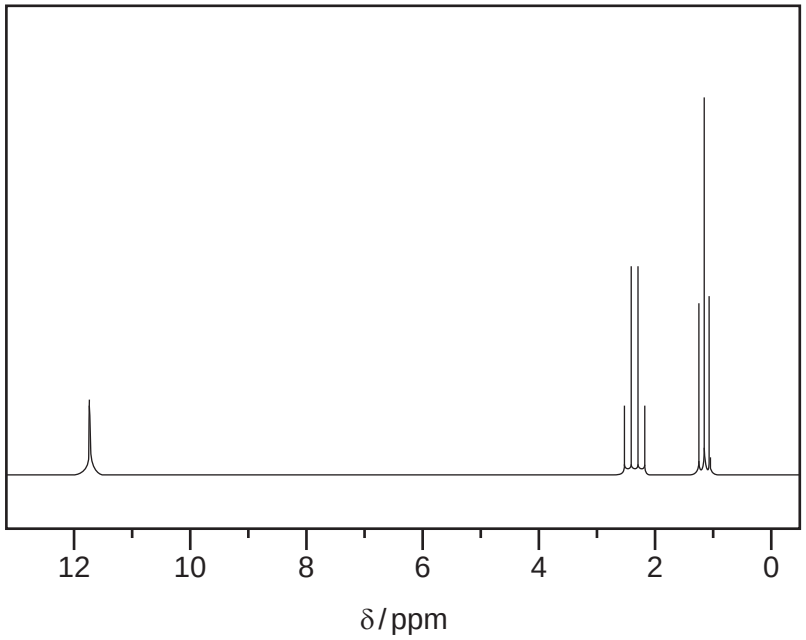
[Total: 12]

3 The combination of mass spectroscopy and NMR spectroscopy provides a powerful method of analysis for organic compounds.

(a) The mass spectrum of a compound **G** contains M and M+1 peaks in the ratio of their heights of 74 : 2.5.
Use these data to calculate the number of carbon atoms present in **G**. Show your working.

[2]

(b) The NMR spectrum of compound **G** is shown.



(i) Use the *Data Booklet* and your knowledge of NMR spectroscopy to identify the type of proton responsible for each of the three absorptions.

δ / ppm	type of proton
1.1	
2.2	
11.8	

(ii) The addition of D_2O causes one of these absorptions to disappear.
Explain why this happens and state which absorption is affected.

.....

.....

(iii) Draw the structural formula of **G**.

[6]

(c) Several structural isomers of **G** exist.

(i) Draw the structural formula of an isomer of **G** with only two absorptions in its NMR spectrum.

(ii) Use the *Data Booklet* to suggest where these absorptions would occur.

peak	δ / ppm
1	
2	

[3]

[Total: 11]

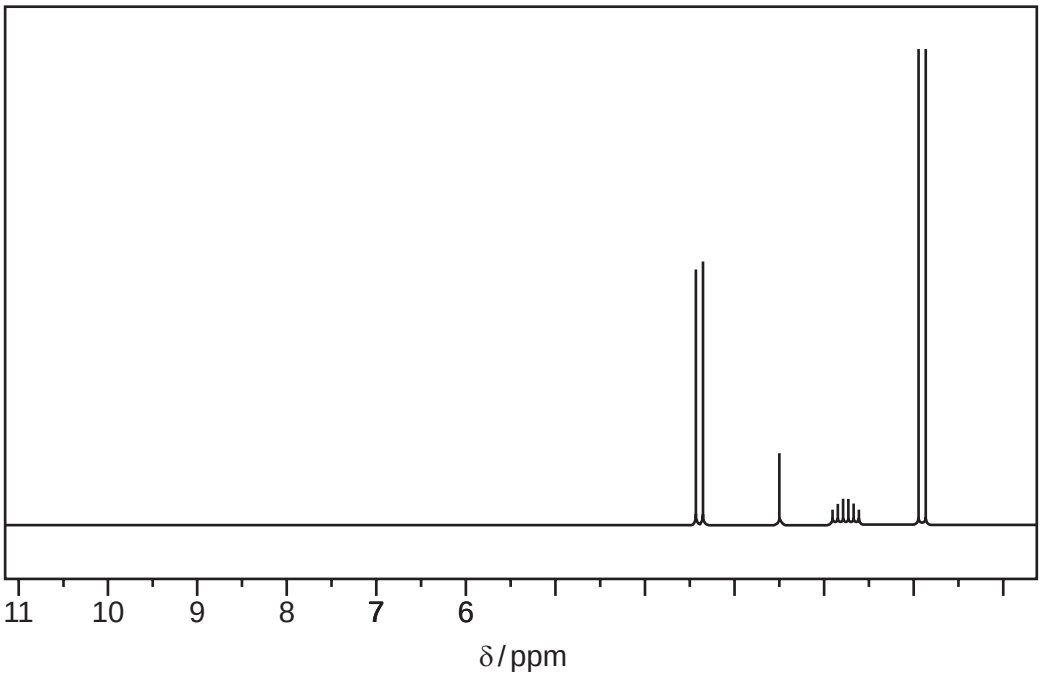
4 **T** is a saturated alcohol. It was analysed by mass spectroscopy and NMR spectroscopy.
In the mass spectrum, the molecular ion peak, M, was at an m/e value of 74 and the ratio of the heights of the M and M+1 peaks was 20.4 : 0.9.

(a) Use the ratio of the heights of the M and M+1 peaks to calculate the number of carbon atoms in a molecule of **T**.

(ii) What is the molecular formula of **T**?

molecular formula = ...
[3]

(b) The NMR spectrum of **T** given below shows four absorptions. The absorption at 1.8 ppm is a multiplet and that at 2.5 ppm is a singlet.



(i) Use this information and your answer to **(a)(ii)** to deduce the structure of **T**.

T

(ii) Describe and explain which type of proton is responsible for each of the absorptions.

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.....

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.....

(iii) The absorption at 1.8 ppm is a multiplet and that at 2.5 is a singlet.
State and explain the splitting patterns of the other absorptions, at 0.9 and 3.4 ppm.

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(iv) Describe and explain how the NMR spectrum of **T** dissolved in D_2O would differ from the one shown.

.....

.....

.....

[9]

[Total: 12]

5 The techniques of mass spectrometry and NMR spectroscopy are useful in determining the structures of organic compounds.

(a) The three peaks of highest mass in the mass spectrum of organic compound **L** correspond to masses of 142, 143 and 144.
The ratio of the heights of the M : M+1 peaks is 43.3 : 3.35, and the ratio of heights of the M : M+2 peaks is 43.3 : 14.1.

(i) Use the data to calculate the number of carbon atoms present in **L**.

(ii) Explain what element is indicated by the M+2 peak.

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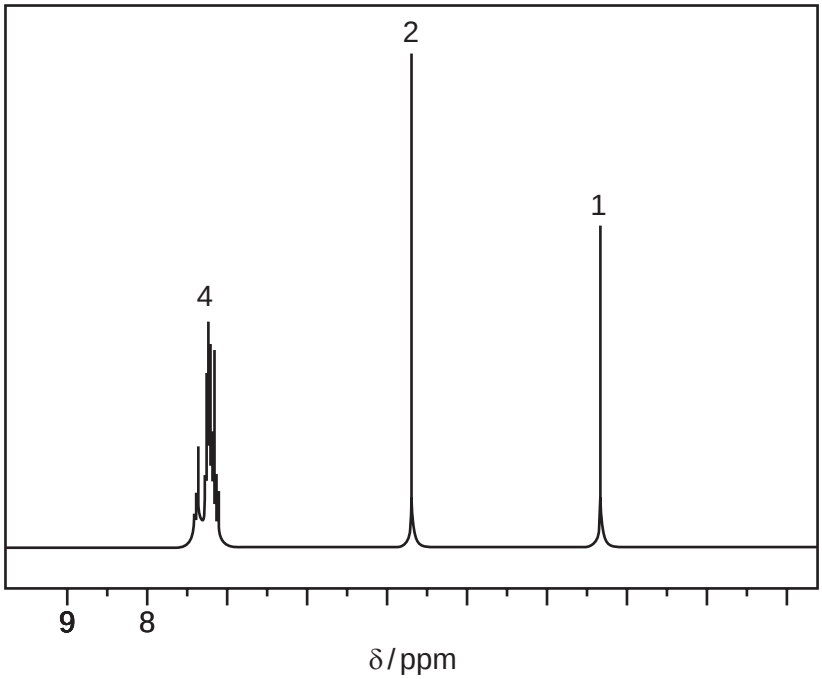
Compound **L** reacts with sodium metal. The NMR spectrum of compound **L** is given below.



(iii) What does the NMR spectrum tell you about the number of protons in **L** and their chemical environments?

.....

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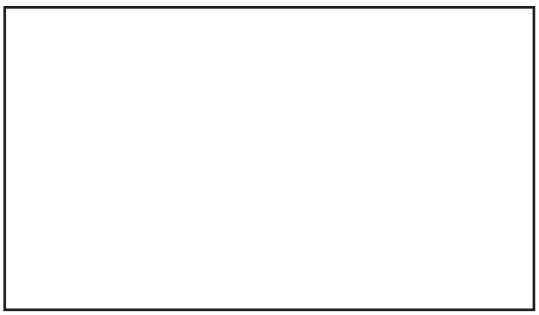
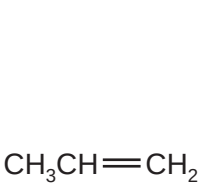
(iv) Use the information given and your answers to **(i)**, **(ii)** and **(iii)** to deduce a structure for **L**.
Explain how you arrive at your answer.

structure of **L**

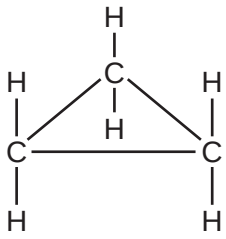


[7]

(b) The molecular formula C_3H_6 represents the compounds propene and cyclopropane.



propene



cyclopropane

(i) Suggest **one** difference in the fragmentation patterns of the mass spectra of these compounds.

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(ii) Suggest **two** differences in the NMR spectra of these compounds.

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.....

[3]

[Total: 10]

6 Instrumental analysis plays an increasingly important role in modern chemistry. Two important techniques are NMR spectroscopy and X-ray crystallography.

(a) Both techniques use part of the electromagnetic spectrum.
Which technique uses radiation with the longer wavelength, and in which part of the spectrum is it found?

.....

[1]

(b) NMR spectroscopy provides detailed information about protons, but X-ray crystallography is unable to detect them. Explain these facts.

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[2]

(c) The protein found in hair contains the amino acid cysteine, $C_3H_7SNO_2$. Crystalline cysteine was examined using X-ray crystallography. State which atom produced the strongest reflection, explaining your answer.

.....

.....

[1]

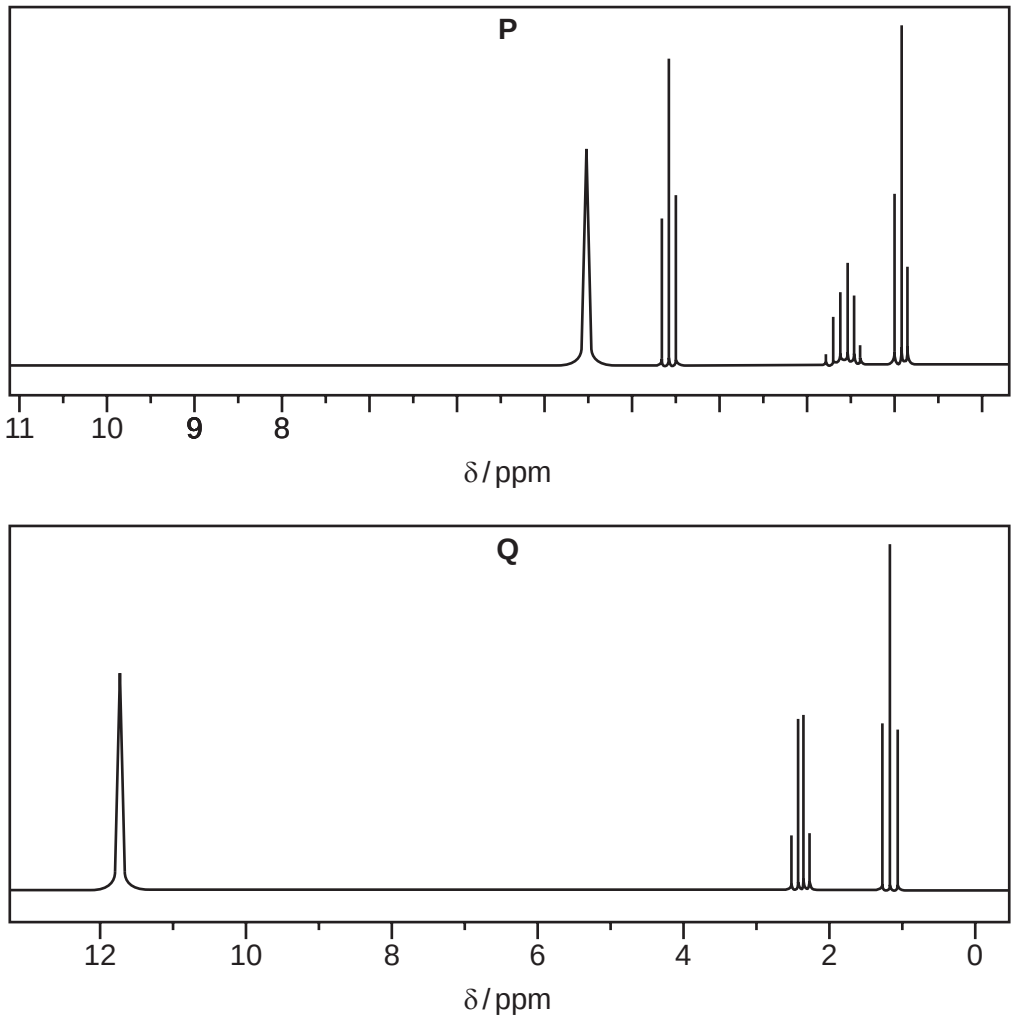
(d) Compound **P** is an alcohol that can be converted into compound **Q** in the following reaction sequence.

$$\mathbf{P} \rightarrow C_xH_6O \rightarrow \mathbf{Q}$$

Spectral analyses of **P** and **Q** were carried out.

(i) The mass spectrum of **P** shows an M : M+1 peak ratio of 4.5 : 0.15.
Calculate the number of carbon atoms in **P**.

The NMR spectra of **P** and **Q** are shown below.



(ii) In the spectrum of **P**, clearly label the peak due to the –OH group with an **X**.

(iii) State how many different proton environments are present in compound **Q**.

.....

(iv) What evidence is there in these spectra that **P** is a primary rather than a secondary alcohol?

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.....

(v) Draw a structure for **Q**.

[6]

[Total: 10]