Mass Spectrometry

Question Paper 2

Level	International A Level
Subject	Chemistry
Exam Board	CIE
Topic	Analytical techniques
Sub-Topic	Mass Spectrometry
Paper Type	Theory
Booklet	Question Paper 2

Time Allowed:	**74 minutes**
Score:	**/61**
Percentage:	**/100**

Grade Boundaries:

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

1 DNA fingerprinting has become an important analytical technique, largely due to its use in 'screening' crime suspects. It also has a range of applications in modern analysis including determining family links, medicine and archaeology.

(a) DNA fingerprinting uses an analytical technique you have studied. What is the name of that technique?

.....

(ii) In order to carry out DNA fingerprinting, the DNA must first be broken down into shorter lengths of polynucleotides. How is this accomplished?

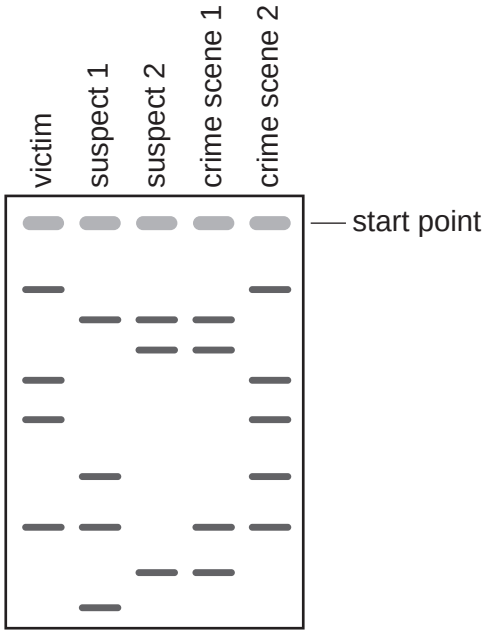
.....

(iii) What part of the DNA fragments enables them to move in an electric field?

.....

[3]

(b) The DNA fingerprints shown were obtained from a crime scene. DNA samples were recovered from two rooms in the house where the crime took place. The victim's DNA and that of two possible suspects were included in the analysis.



(i) Indicate with an **X** on the diagram, which lines from suspect 1 and from suspect 2 **cannot** distinguish which of them was present in the house.

(ii) Based on this evidence one suspect was arrested. Which suspect would you expect this to be? Explain your reasoning.

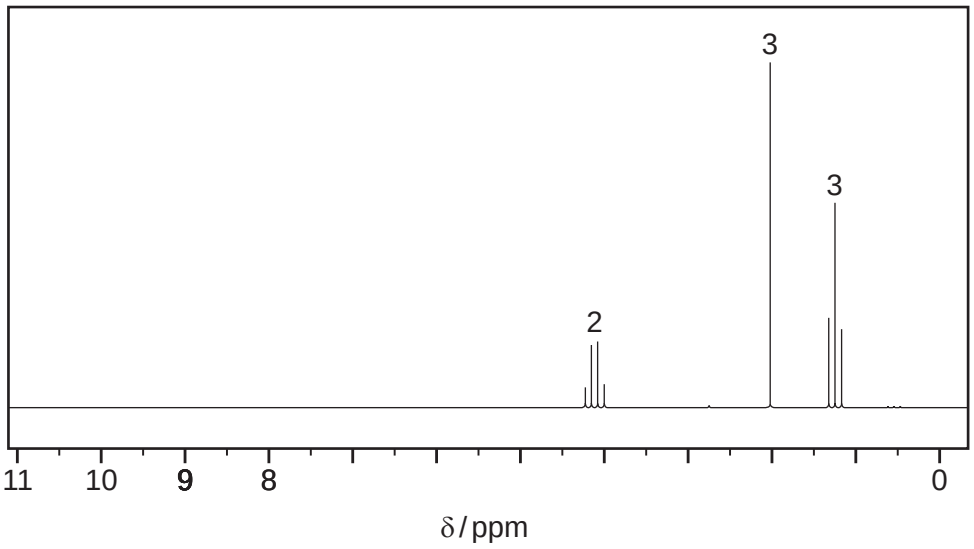
.....

.....

[2]

(c) A sample of a liquid, **P**, was found at the scene of the crime and was analysed using mass spectrometry and NMR spectroscopy.

The mass spectrum has M and M+1 peaks in the ratio of 5.1: 0.22 with the M peak at *m*/*e* = 88.
The NMR spectrum is shown



Use the data to suggest a structure for **P**, explaining your answer.

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.....

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.....

.....

structure of **P**

[5]

[Total: 10]

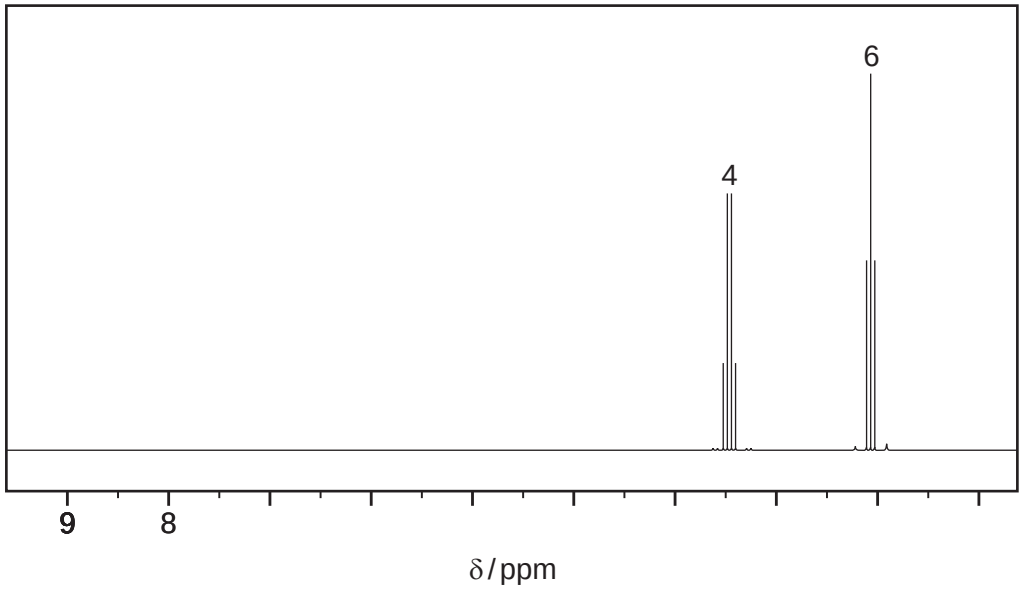
2 Although the chemical reactions of compounds remain important pointers to their functional groups, instrumental techniques such as mass spectrometry and NMR spectroscopy are increasingly used to determine molecular structures.

(a) Compound **J** was analysed using these two techniques with the following results.

The mass spectrum showed that

- the M peak was at *m/e* 86,
- the ratio of heights of the M and M+1 peaks was 23.5 : 1.3.

The NMR spectrum is shown below.



(i) Use the data to determine the number of carbon and hydrogen atoms present in **J**, showing your working.

(ii) Use the information given above and your answer to **(i)** to identify the other element present in **J**.

.....

(iii) Determine the structure of **J**, explaining how you reach your conclusion.

structure of **J**

explanation .....

.....

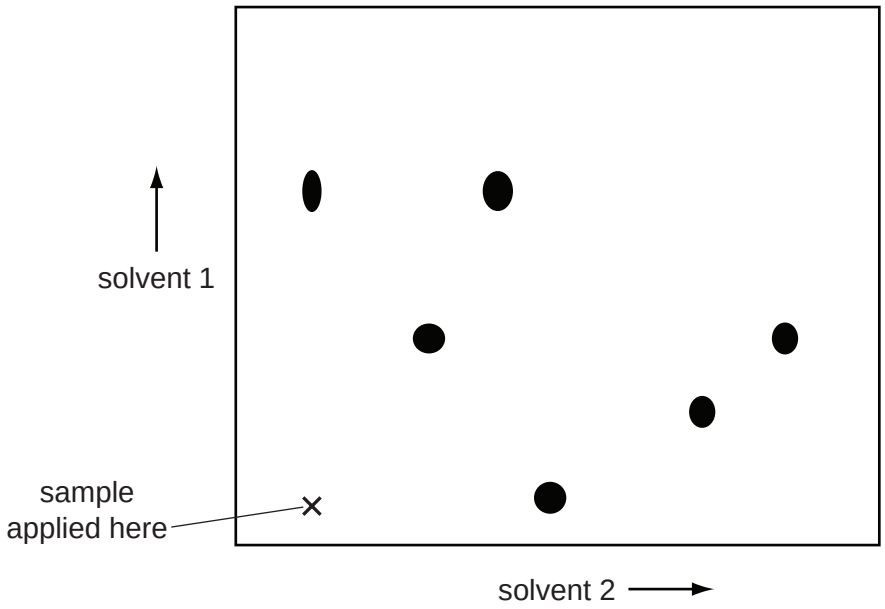
[5]

(b) Chromatography is another important analytical technique used in chemistry.

(i) Paper, thin-layer and gas-liquid chromatography rely on different physical methods to separate the components in a mixture. Complete the table indicating the appropriate method on which the technique is based.

technique	physical method
paper chromatography	
thin-layer chromatography	
gas-liquid chromatography	

In paper chromatography, better separation may be achieved by running the chromatogram in one solvent, then turning the paper at right angles and running it in a second solvent. The chromatogram below was produced in this way.



(ii) How many spots were visible **before** solvent 2 was used?

.....

(iii) Ring the spot that did **not** move in solvent 2.

(iv) How many spots travelled further in solvent 2 than they did in solvent 1?

.....

[5]

[Total: 10]

3 **(a)** NMR spectroscopy and X-ray crystallography are two techniques that use electromagnetic radiation to look at the structures of large molecules.

For each technique state the sub-atomic particle involved, and explain how this particle interacts with the radiation.

NMR.....

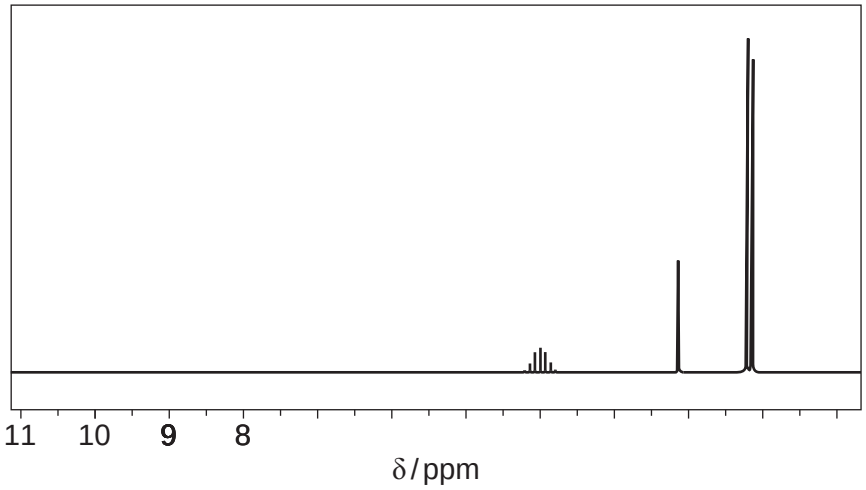
.....

X-ray .....

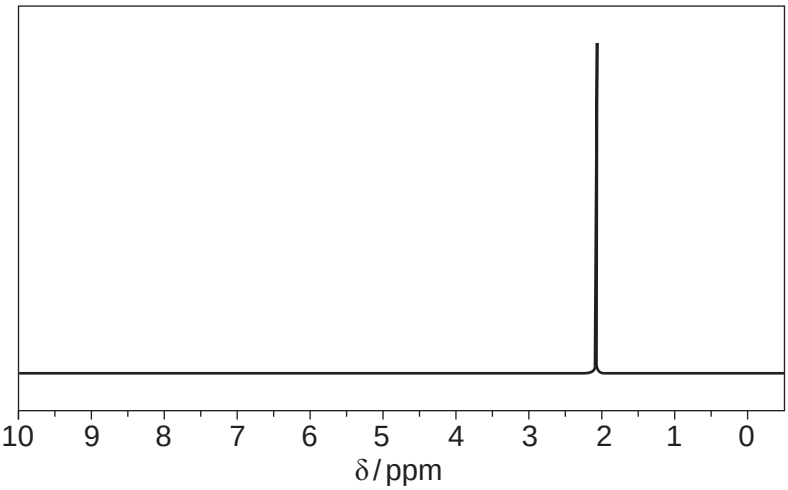
.....

[4]

(b) The two NMR spectra **1** and **2** were obtained before and after an alcohol, **Y**, was oxidised to give compound **Z**. The numbers of hydrogen atoms responsible for each peak have **not** been shown. All the peaks have been shown.



1



2

(i) State which spectrum, **1** or **2**, was produced by the alcohol, giving a reason for your answer.

spectrum .....

reason .....

.....

(ii) The mass spectrum of **Y** showed an M : M + 1 peak ratio of 17.6:0.6.
Use this and other information in the question to suggest the identities of both **Y** and **Z**.

(iii) Draw a displayed formula for **Y** in the box provided

Y is

(iv) Explain why the NMR spectrum of **Z** only shows one peak.

.....

.....

[7]

[Total: 11]

4 This question is about the modern techniques of analysis which may be used to determine molecular structures.

(a) In X-ray crystallography X-rays are diffracted by the electron clouds surrounding individual atoms in the structure.

(i) What useful information is provided by X-ray crystallography?

.....

.....

(ii) Why cannot hydrogen atoms in a structure be detected by this technique?

.....

[2]

(b) Suggest how structures of complex molecules such as enzymes, derived from X-ray crystallography, can help explain their biochemical behaviour.

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.....

..... [2]

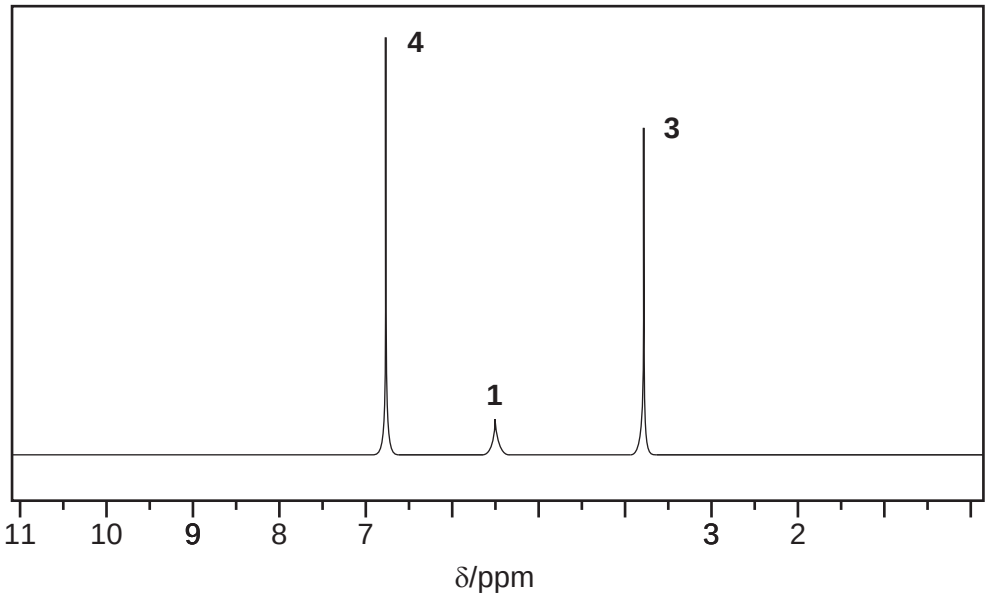
(c) NMR spectroscopy, in contrast to X-ray crystallography, is frequently used to examine protons in organic molecules.

(i) What feature of protons enables their detection by NMR spectroscopy?

.....

(ii) The NMR spectrum below was obtained from a compound **X**, $C_xH_yO_z$. In the mass spectrum of the compound, the M : M+1 ratio was found to be 25:2.

Determine the values of x, y and z in the formula of **X** and deduce a possible structure for the compound, explaining how you arrive at your conclusion.



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Possible structure of **X**

[6]

[Total:10]

5 The technology of DNA fingerprinting has enormously advanced scientific identification techniques in medicine, crime detection and archaeology in recent years.

(a) **(i)** In order to prepare a DNA sample for analysis, the DNA is treated with restriction enzymes. What do restriction enzymes do?

.....

.....

(ii) What is the next stage in DNA analysis, after the treatment with restriction enzymes?

.....

(iii) How are the DNA fragments made visible?

.....

[3]

(b) NMR and X-ray crystallography have made significant contributions to our knowledge of the structure of proteins and, in the pharmaceutical industry, how drugs react with target proteins.

(i) Suggest an advantage of **each** technique in helping to determine protein structure.

.....

.....

.....

(ii) MRI scanning is a medical technique based on NMR spectroscopy. It is particularly useful for looking for tumours in healthy tissue.

Suggest how this technique can distinguish tumour tissue from healthy tissue.

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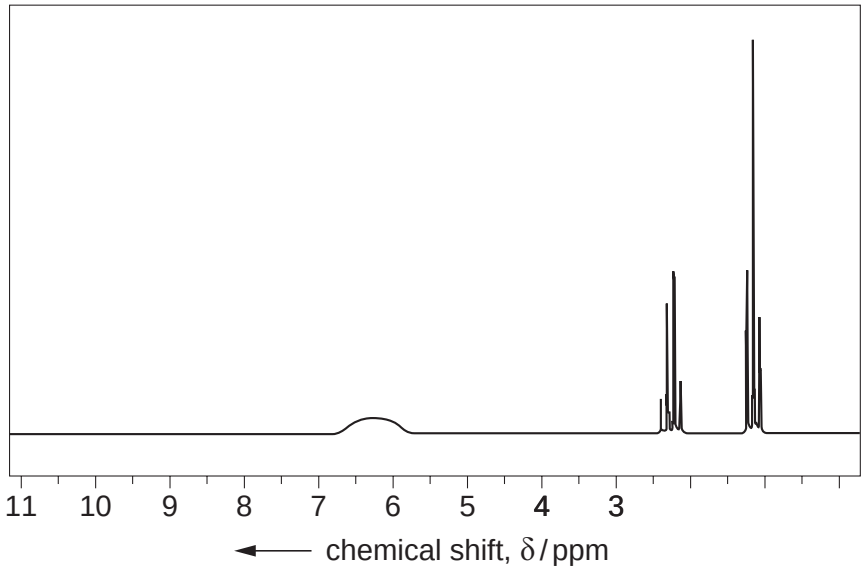
.....

[3]

(c) A saturated molecule of formula C_xH_yNO was subjected to analysis by mass spectrometry and NMR spectroscopy. In the mass spectrum of the compound, the M peak was at *m/e* 73 and the ratio of the heights of the M:M+1 peak was 48 : 1.7.

(i) Using the data from the mass spectrum, determine the values of *x* and *y* in the formula of the compound.

(ii) Use the data from **(i)** together with the NMR spectrum below to deduce a structure for the compound, explaining how you arrive at your answer.



[4]

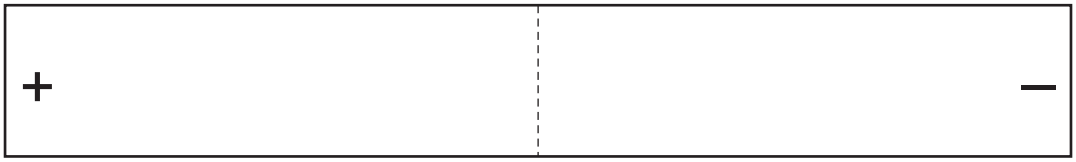
[Total: 10]

6 The analysis of a protein may be carried out by breaking it down into its amino acids. These can then be separated by a process called electrophoresis.

(a) The structures of glycine, lysine and glutamic acid at pH 7 are shown.

glycine	$H_3N^+CH_2CO_2^-$
lysine	$H_3N^+CH(CH_2CH_2CH_2CH_2NH_3^+)CO_2^-$
glutamic acid	$H_3N^+CH(CH_2CH_2CO_2^-)CO_2^-$

Draw and label three circles on the chart below to indicate the likely position of each of these amino acids after electrophoresis of a solution containing these amino acids in a buffer at pH 7.



[3]

(b) Some organic compounds have very different solubilities in water and in organic solvents such as hexane. They may be extracted from an aqueous reaction mixture by shaking the mixture with portions of hexane and separating the two layers.
The process of distribution of a compound between two solvents is called *partition*.

(i) State what is meant by the term *partition coefficient*.

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(ii) One of the concerns about organic pollutants, such as pesticide residues, is that they can enter the food chain and become concentrated in human breast milk. Explain how this can happen.

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[3]

(c) Propene was treated with bromine in the presence of chloride ions and the product analysed using mass spectrometry.

A group of peaks was found in the range *m*/*e* 156–160 with the following relative heights.

m/*e*	relative height
156	3
158	4
160	1

(i) Identify the species responsible for each of these peaks.

156 .....

158 .....

160 .....

A large peak was present in the spectrum with a *m*/*e* value of less than 20.

(ii) Suggest the *m*/*e* value for the peak and the species that produced it.

m/*e* .....

species .....

[4]

[Total: 10]