Hydrogen NMR

Question Paper 2

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

Time Allowed:	**36 minutes**
Score:	**/30**
Percentage:	**/100**

Grade Boundaries:

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

1 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?

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[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.

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[1]

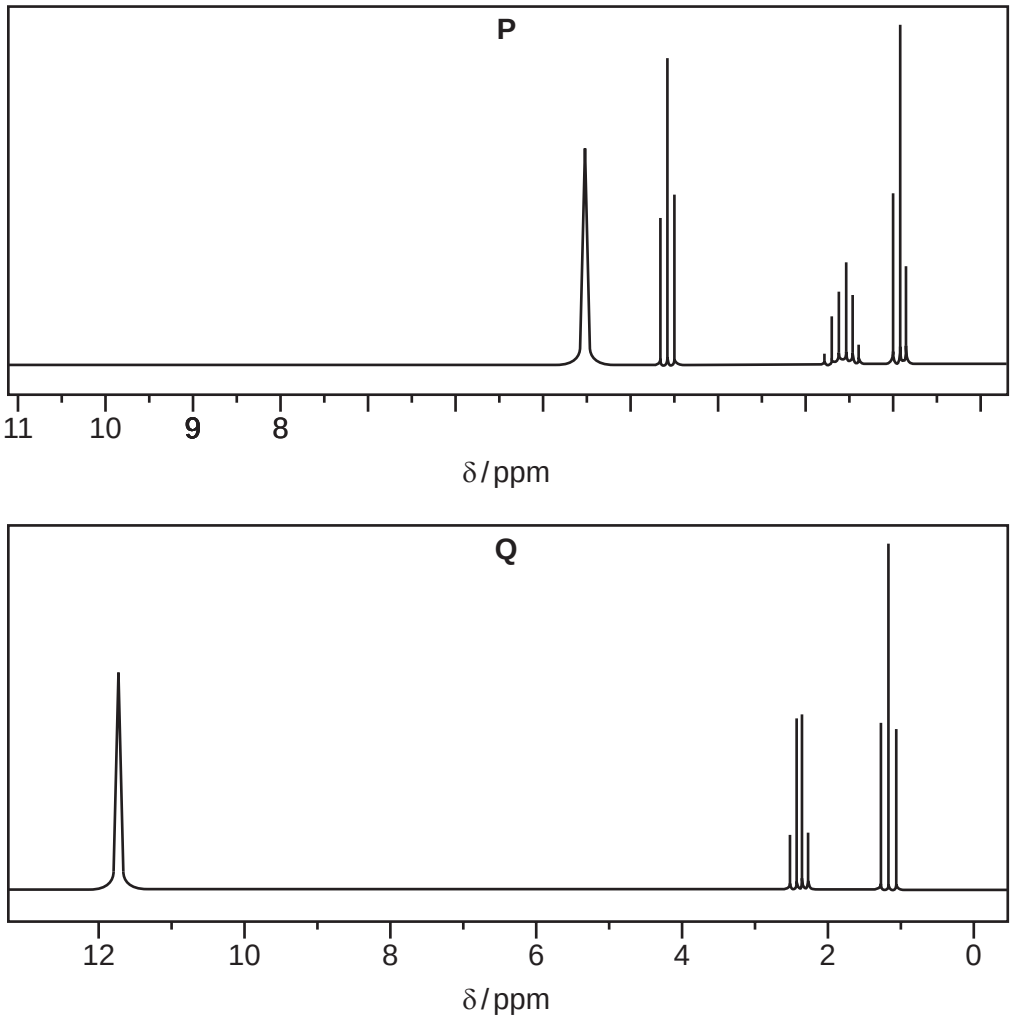
(d) Compound **P** is an alcohol that can be converted into compound **Q** in the following reaction sequence.

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

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**.

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(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]

2 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?

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

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

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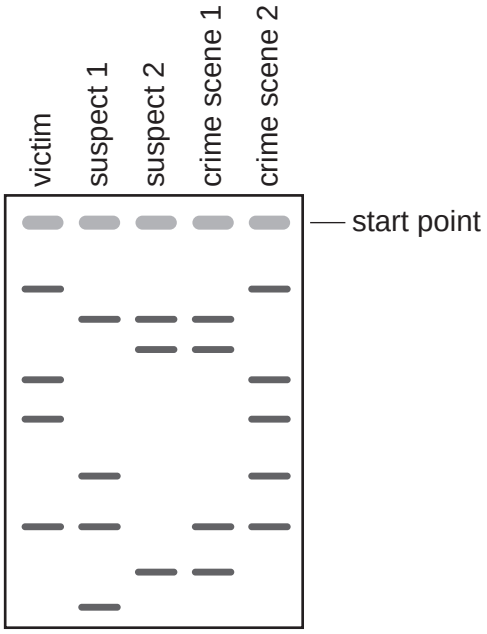
[3]

(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.

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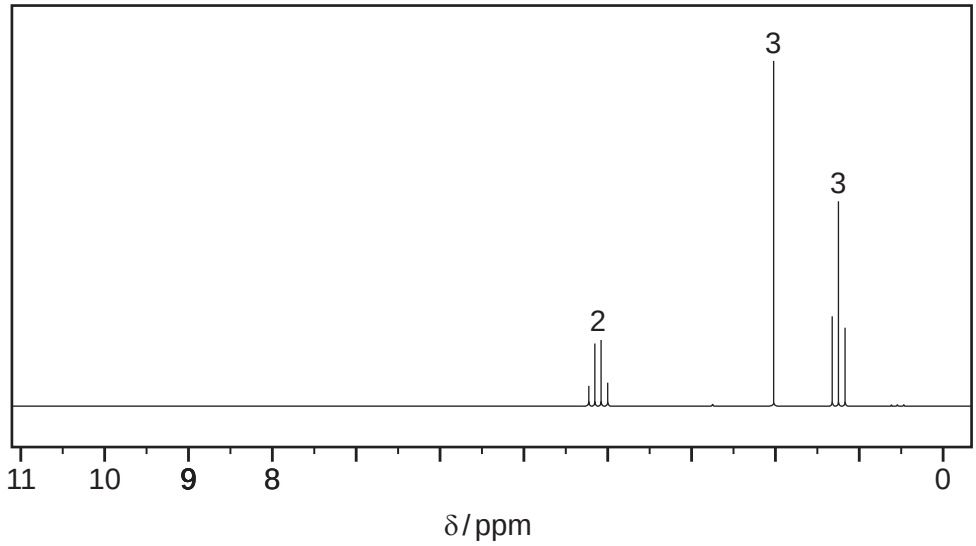
[2]

(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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structure of **P**

[5]

[Total: 10]

3 A range of modern analytical techniques has made the identification of molecules, and atoms in compounds, much more rapid than traditional laboratory analysis.

(a) One instrumental technique is NMR spectroscopy, which uses the fact that under certain conditions protons can exist in two different energy states.
Explain how these different energy states arise.

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.....[2]

(b) When methanol, CH_3OH, is examined using NMR spectroscopy, it absorbs at two different frequencies. Explain why, and predict the relative areas of the two peaks.

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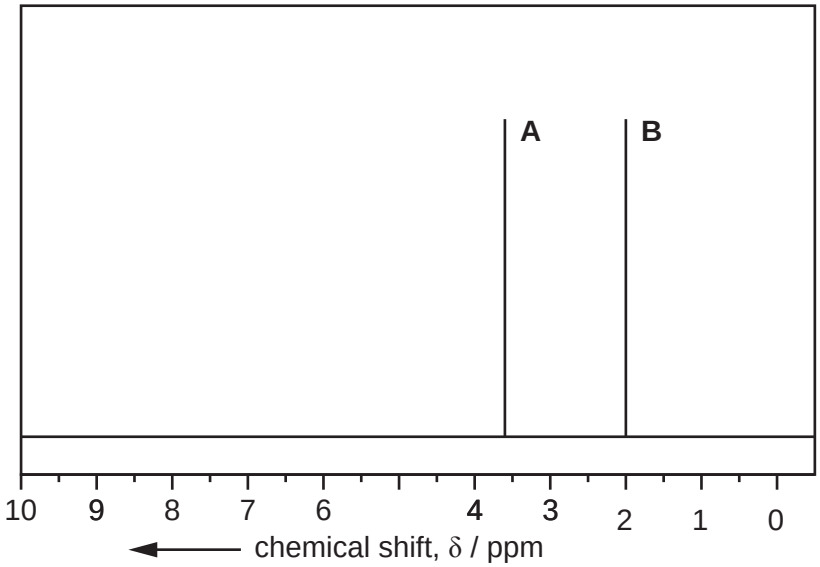
.....[2]

(c) The NMR spectrum below is that of one of three possible isomers of molecular formula $C_3H_6O_2$.



The compound could be propanoic acid, methyl ethanoate or ethyl methanoate.

(i) In the boxes provided, draw the structures of the three compounds.

propanoic acid	methyl ethanoate	ethyl methanoate

(ii) Explain which compound produced the spectrum shown, indicating which protons are responsible for each of the peaks **A** and **B**.

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(iii) The NMR spectrum of another of the compounds has a peak at δ11.0.
State which compound this would be, and identify the proton(s) responsible for this peak.

compound .....

proton(s) .....

[4]

(d) X-ray crystallography is a technique used to identify the relative positions of atoms in a crystal of a compound.

(i) What further information about organic macromolecules can be deduced by the use of X-ray crystallography?

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(ii) Which atoms cannot be located by X-ray crystallography?

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[2]

[Total: 10]