Hydrogen NMR
Question Paper 1

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

Time Allowed: 65 minutes

Score: /54

Percentage: /100

Grade Boundaries:

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

1 NMR and X-ray crystallography are two important analytical techniques which can be used to study the structure and function of molecules.

(a) Nuclear magnetic resonance, NMR, arises because protons possess spin which generates a small magnetic moment. When an external magnetic field is applied the protons can align with or against the external field. If they are given a small amount of energy in the radio frequency range each can be 'promoted' so that their magnetic moment opposes the external field.
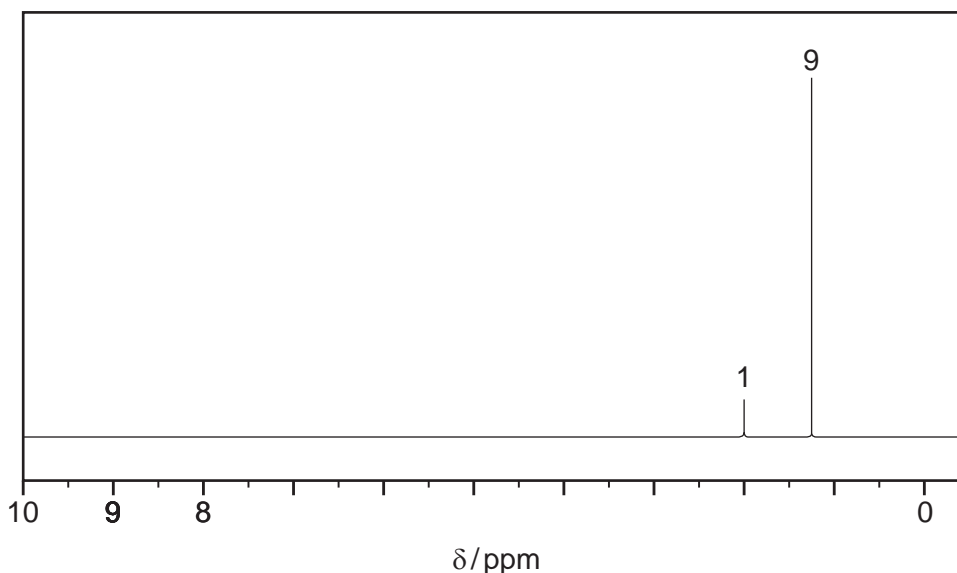
Two factors can influence the energy required for this promotion. What are they?

(i) ....

(ii) ....

[2]

(b) A compound, **J**, has the formula $C_4H_{10}O$. The NMR spectrum of **J** is shown.

δ/ppm

(i) Indicate the groups responsible for each peak and hence deduce the structure of **J**.

peak at $1.26\,\delta$ ....   peak at $2.0\,\delta$ ....

structure of **J**

(ii) There are three other isomers of **J** containing the same functional group as **J**. Draw the structures of two of these three isomers and indicate how many different chemical shifts each would show in its NMR spectrum.

isomer 1   isomer 2

number of groups of peaks .... number of groups of peaks ....

[6]

(c) X-ray crystallography can be useful in gathering information about the structure of large organic molecules, such as nucleic acids.

(i) Which element will show up most strongly in the X-ray crystallography of a nucleic acid? Explain your answer.

....

....

(ii) X-ray crystallography will **not** detect hydrogen atoms. Explain why this is so.

....

....

[2]

[Total: 10]

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 [1] to X-rays.

....

.... [1]

(b) The NMR spectrum below was obtained from an organic liquid, **P**, which contains five carbon atoms per molecule.
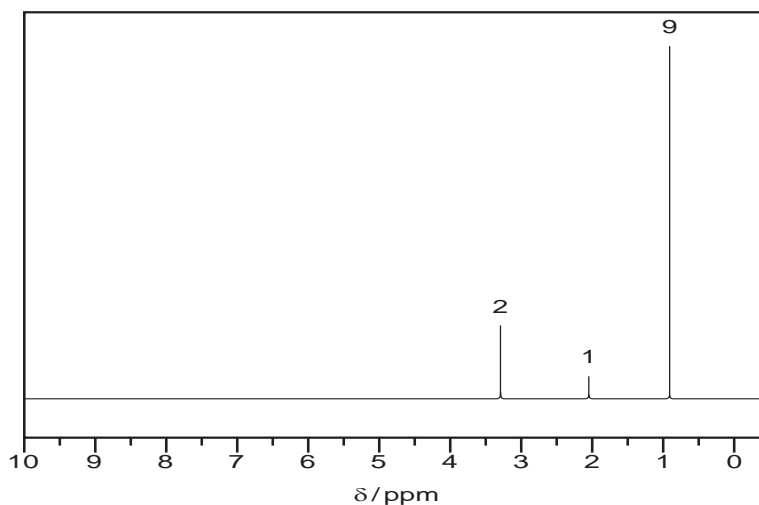
(i) How many protons are present in one molecule of **P**? Explain your answer.

number of protons ....

....

.... [1]

(ii) When a little D_2O is added to **P**, the absorption at $\delta 2.0$ disappears.

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

....

....

.... [2]

(iii) What does the absorption at $\delta 0.9$ tell you about the adjacent carbon atom?

....

.... [1]

(iv) What group(s) is/are responsible for the absorption at $\delta 0.9$?

.... [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 fiv e 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 **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
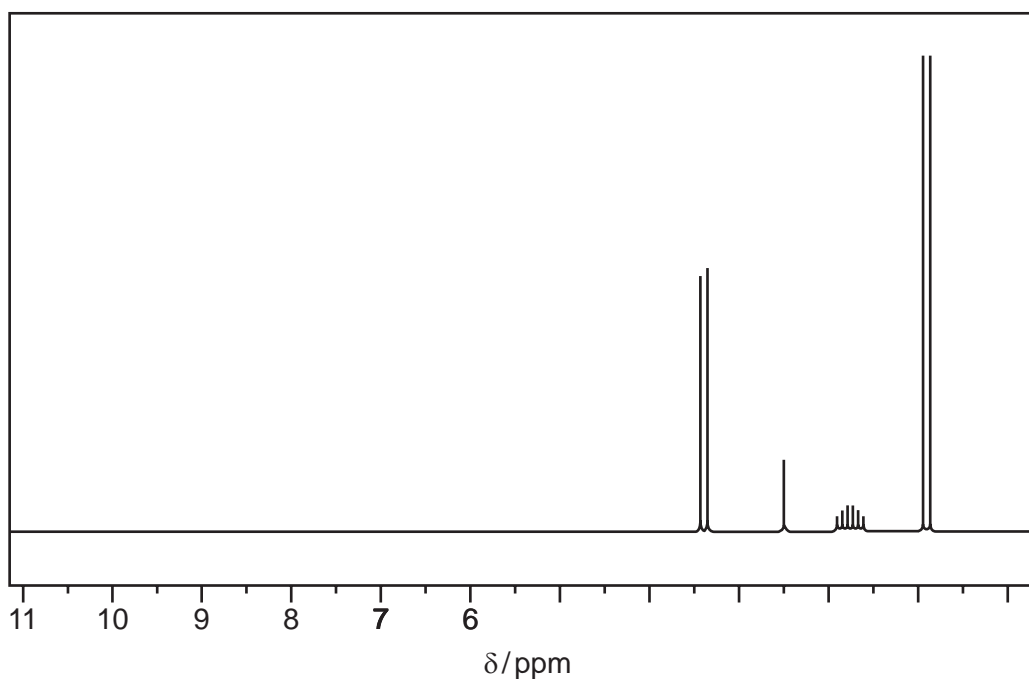heights of the M and M+1 peaks was 20.4 : 0.9.

(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**.

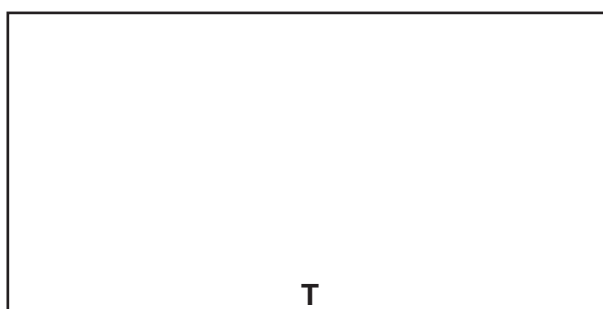**(ii)** What is the molecular formula of **T**?

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.

δ/ppm

(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.

....

....

....

....

(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.

....

....

....

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

....

....

....

[9]

[Total: 12]

4 **(a)** Analysis of a sample of DNA showed that 33% of the nitrogenous bases present was guanine. Calculate the percentages of the **other** bases in this sample of DNA.

adenine ....% cytosine ....% thymine ....% [2]

(b) Many drug molecules are chiral, but are often produced as a mixture of optical isomers.

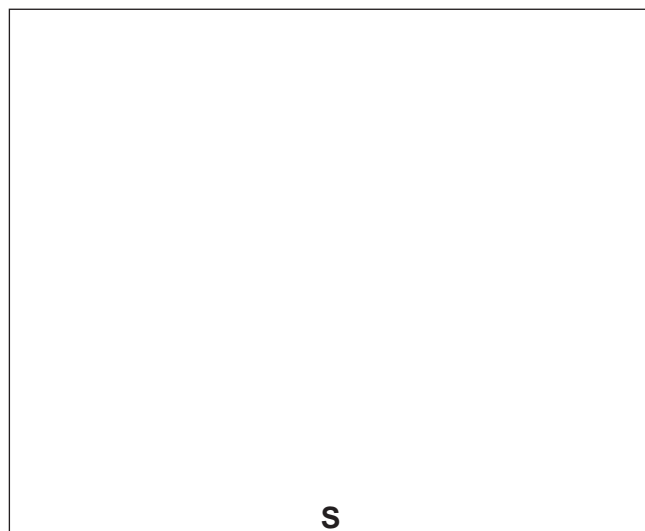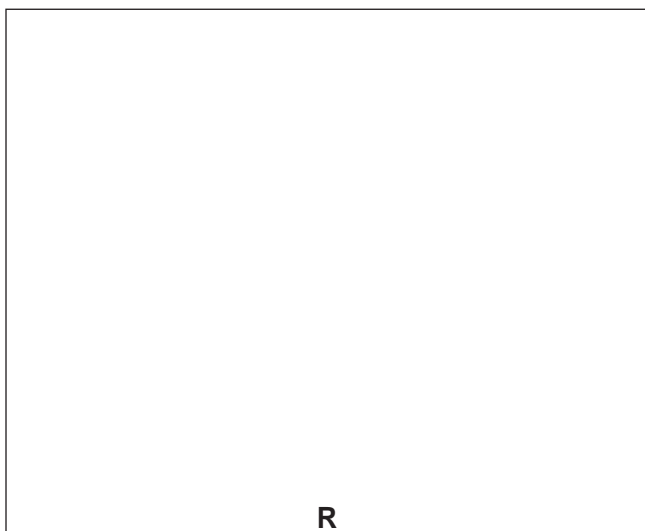**(i)** Suggest why a larger mass of the mixture is required than of a single optical isomer.
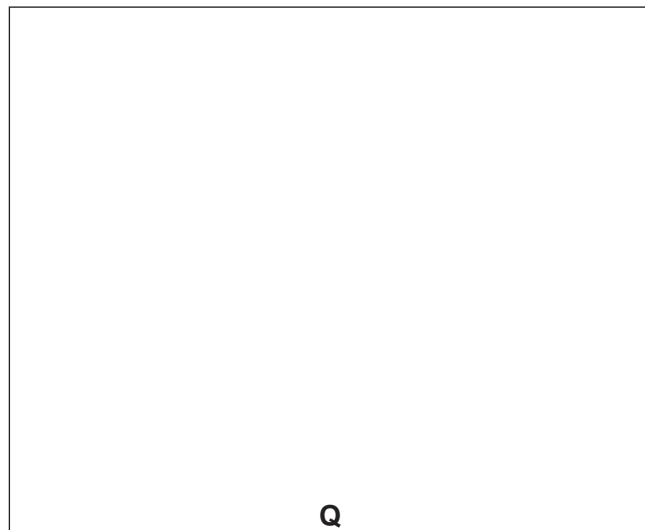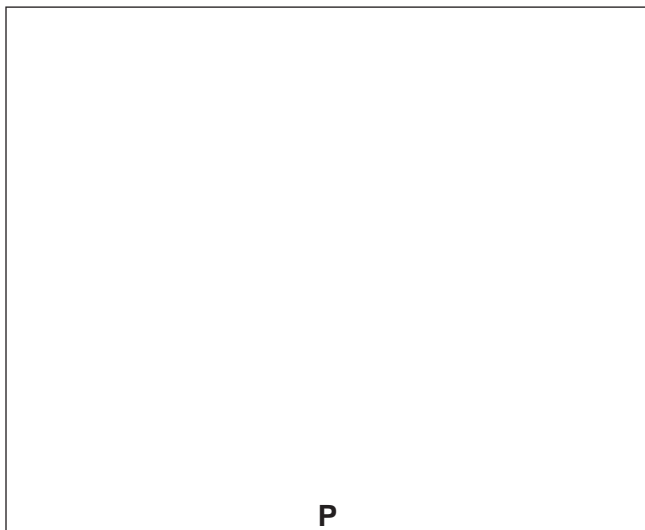
....

....

(ii) Suggest a problem that might arise as a result of taking a mixture of optical isomers.

....

....
[2]

(c) There are four structural isomers with the molecular formula $C_5H_{10}O$ that are aldehydes.

(i) Draw the structures of these aldehydes.

P

Q

R

S

(ii) The NMR spectrum of **one** of these isomers contains **four** absorptions.
Which isomer **P**, **Q**, **R** or **S** gives this spectrum?

isomer ....

(iii) Predict the number of absorptions that would be given by each of the other three isomers.

isomer letter (**P**, **Q**, **R** or **S**)	number of absorptions

[6]

[Total: 10]

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.
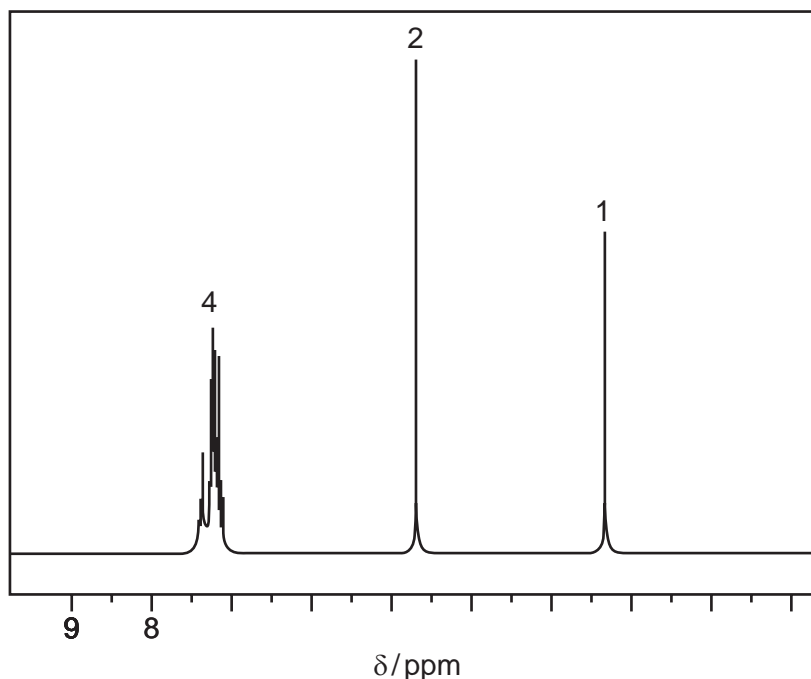The ratio of the heights of the M:M+1 peaks is 43.3:3.35, and the ratio of heights of the M:M+2 peaks is 43.3:14.1.

(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.

....

....

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?
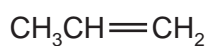
....

....

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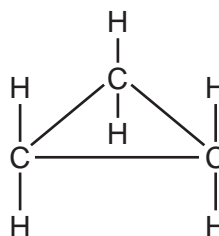**Explain** how you arrive at your answer.

structure of **L**

[7]

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

$$CH_3CH=CH_2$$

propene   cyclopropane

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

....

....

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

....

....

....

[3]

[Total: 10]