

- 8 (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.....

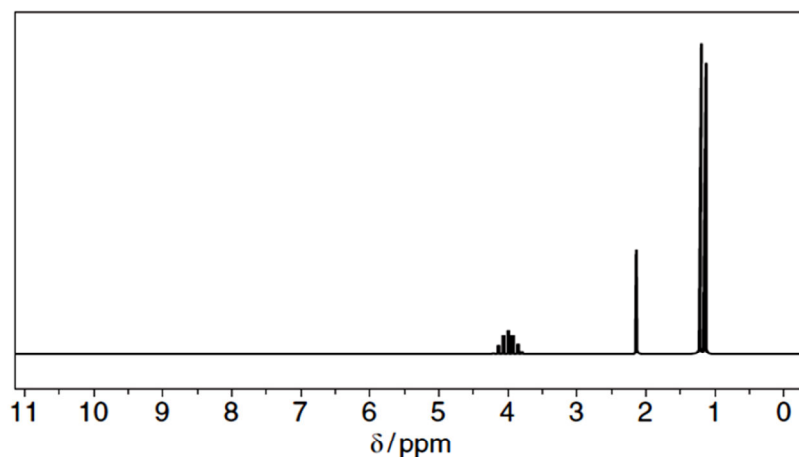
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X-ray

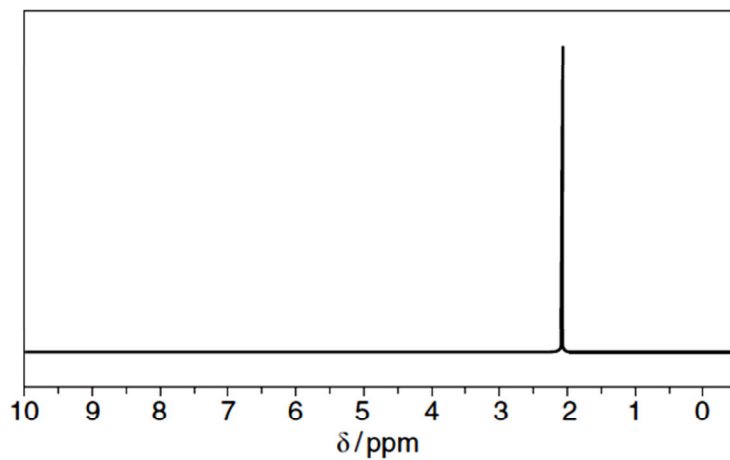
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[4]

- (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

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- (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.

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[7]

[Total: 11]

(b) NMR spectroscopy is a very important analytical technique for use with organic compounds.

(i) Why is NMR spectroscopy particularly useful for organic compounds?

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(ii) Two molecules, propanal and propanone, have the same molecular formula, C_3H_6O . Draw the displayed formula of each compound and explain briefly how NMR spectroscopy can distinguish between the two structures.

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[4]

[Total: 9]

- 9 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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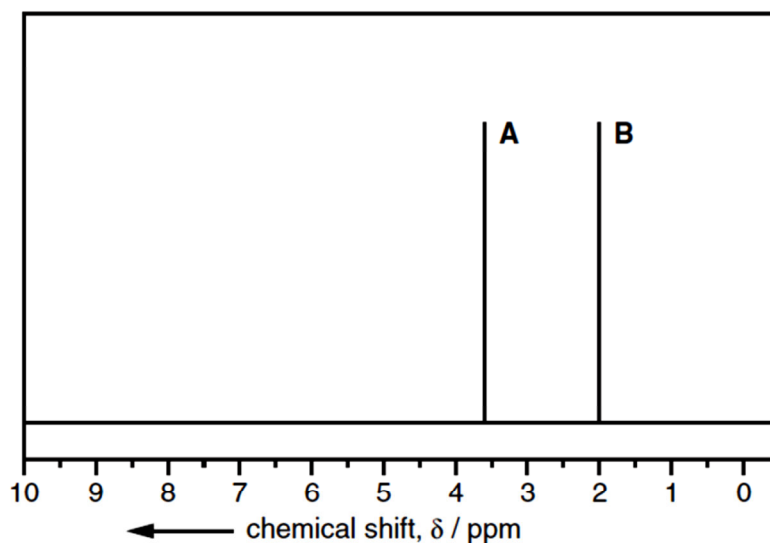
 [2]

- (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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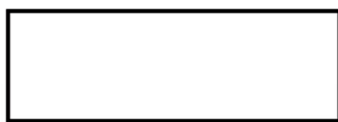
 [2]

- (c) The NMR spectrum below is that of one of three possible isomers of molecular formula $\text{C}_3\text{H}_6\text{O}_2$.



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

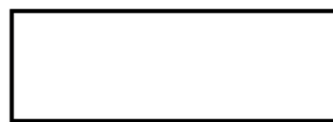
- (i) In the boxes provided, draw the structures of the three compounds.



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 $\delta 11.0$. 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?

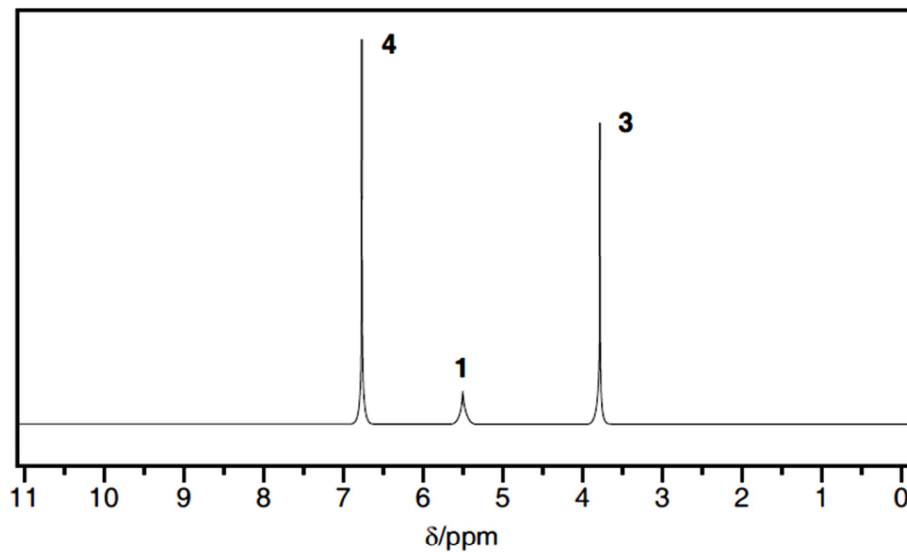
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[2]

[Total: 10]

- (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]

- 9 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?

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

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- (iii) How are the DNA fragments made visible?

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[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.

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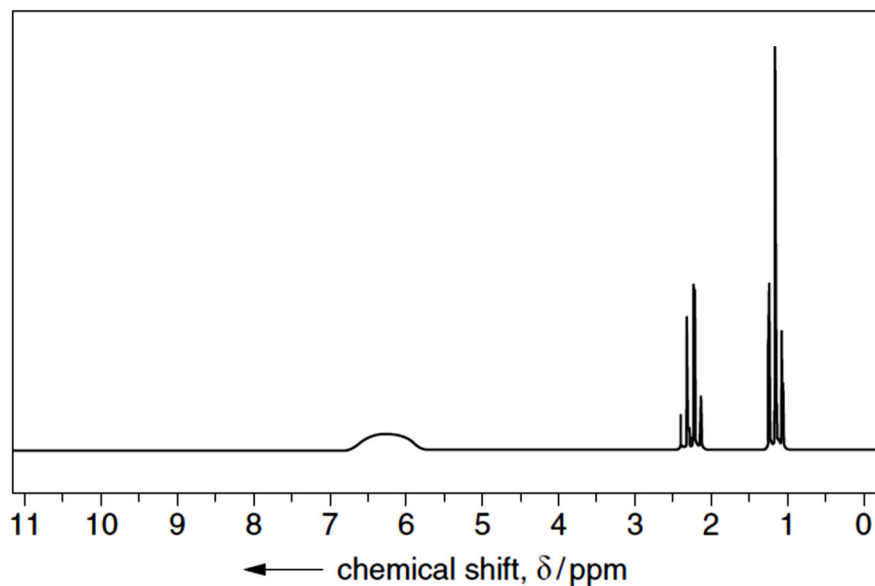
- (ii) MRI scanning is a medical technique based on NMR spectroscopy. It is particularly useful for looking for tumours in healthy tissue.

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.



- 9** Much of the preparation of evidence to solve crimes now relies on instrumental analysis. This question deals with some of the techniques used.

(a) Electrophoresis can be used to separate amino acids produced by hydrolysing proteins. The amino acids are placed in a buffered solution in an electric field. In a solution of given pH, what **two** factors affect the movement of a given amino acid?

(i)

(ii) [2]

(b) Nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry are also used in the detection of certain molecules, particularly those containing hydrogen atoms.

(i) Explain how and why the NMR spectrum of propanal, $\text{CH}_3\text{CH}_2\text{CHO}$, would be different from that of propanone, CH_3COCH_3 , which contains the same atoms.

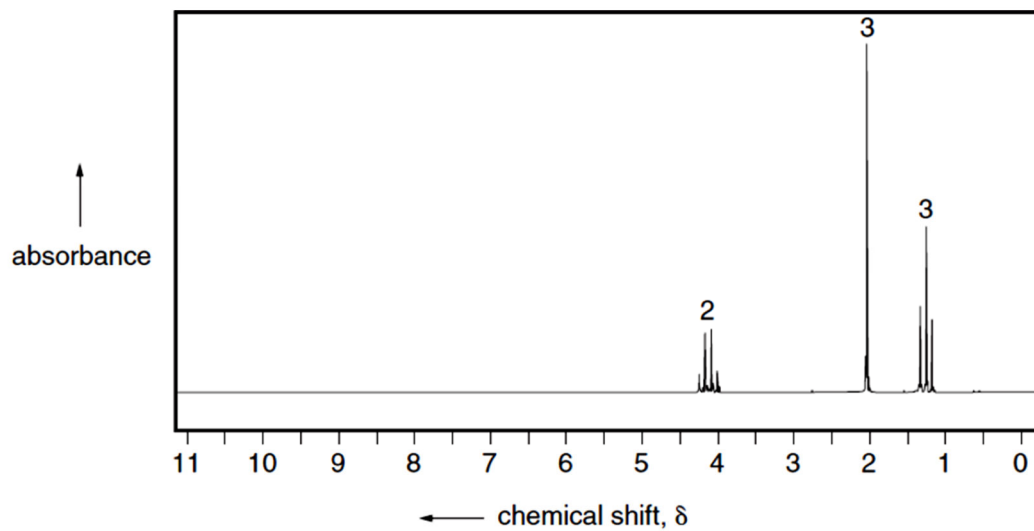
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(ii) Explain how and why the mass spectrum of the two compounds in **(i)** would be different.

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[4]

- (c) The NMR spectrum shown below was obtained from a simple organic molecule, **G**, $C_xH_yO_2$. When a sample of **G** was placed in a mass spectrometer, the ratio of the $M : M+1$ peaks for the molecule was 14.5 : 0.66.



- (i) Calculate how many carbon atoms there are in the molecule.
- (ii) Use the NMR spectrum and the *Data Booklet* to work out the structure of **G**.