

Q1.

- 2 (a) Write an equation showing the reaction that occurs when calcium nitrate, $\text{Ca}(\text{NO}_3)_2$, is heated.

.....[1]

- (b) Describe and explain the trend in thermal stability of the nitrates of the Group II elements.

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.....
.....[3]

- (c) Gently heating ammonium nitrate, NH_4NO_3 , in a test tube produces a mixture of two gases **A** and **B**. No residue remains in the tube.

The mass spectrum of gas **A** contains peaks at m/e (mass number) values of 16, 17 and 18, whereas that of gas **B** has peaks at m/e values of 14, 16, 28, 30 and 44.

- (i) Identify the peaks in the mass spectra, and suggest the molecular formulae of the gases **A** and **B**.

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.....

- (ii) Hence suggest an equation for the thermal decomposition of ammonium nitrate.

..... [5]

[Total: 9]

Q2.

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) At one time, bromomethane, CH_3Br , was widely used to control insect pests in agricultural crops and timber. It is now known to break down in the stratosphere and contribute to the destruction of the ozone layer.

Samples can be screened for traces of bromomethane by subjecting them to mass spectrometry.

- (i) Which peak(s) would show the presence of bromine in the compound?

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- (ii) How could you tell by studying the M and M+2 peaks that the compound contained bromine rather than chlorine?

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[3]

[Total: 9]

Q3.

- 8 A large number of organic compounds are soluble in both water and non-aqueous solvents such as hexane. If such a compound is shaken with a mixture of water and the non-aqueous solvent, it will dissolve in both solvents depending on the solubility in each.

For
Examine
Use

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

.....

.....

- (ii) When 100 cm^3 of an aqueous solution containing 0.50 g of an organic compound **X** was shaken with 20 cm^3 of hexane, it was found that 0.40 g of **X** was extracted into the hexane.

Calculate the partition coefficient of **X** between hexane and water.

- (iii) If **two** 10 cm^3 portions of hexane were used instead of a single 20 cm^3 portion, calculate the total amount of **X** extracted and compare this with the amount extracted using one 20 cm^3 portion.

[5]

- (b) PCBs are highly toxic compounds released into the atmosphere when some plastics are burned at insufficiently high temperatures. In recent years PCB residues have been found in the breast milk of Inuit mothers in northern Canada. Foods, such as oily fish, seal and whale meat, which are high in fat, form an important part of the Inuit diet.

*For
Examiner's
Use*

- (i) Suggest why berries and drinking water are not contaminated by PCBs in the same way that oily fish, seal and whale meat are.

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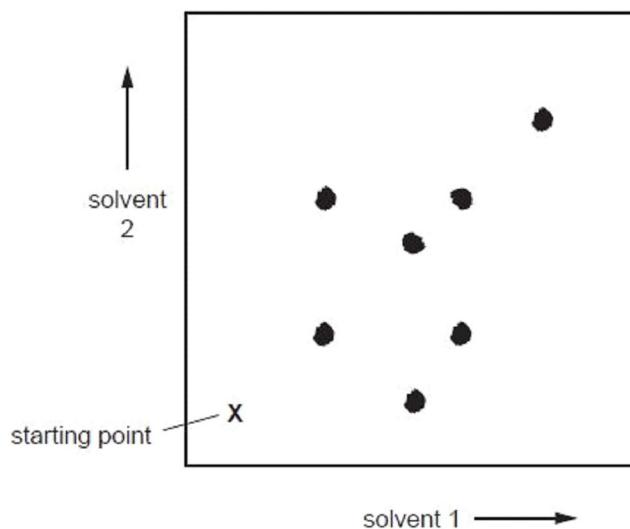
- (ii) Based on the information provided, what can you say about the partition coefficient between fat and water for PCB residues?

.....
.....
.....

[3]

(c) The diagram shows the result of two-way paper chromatography.

For
Examiner's
Use



(i) How many spots were there after the first solvent had been used?

.....

(ii) Circle the spot that moved very little in solvent 2, but moved a greater distance in solvent 1.

(iii) Draw a square around the spot that could be separated from the rest by using **only** solvent 1.

[3]

[Total: 11]

Q4.

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

For
Examiners
Use

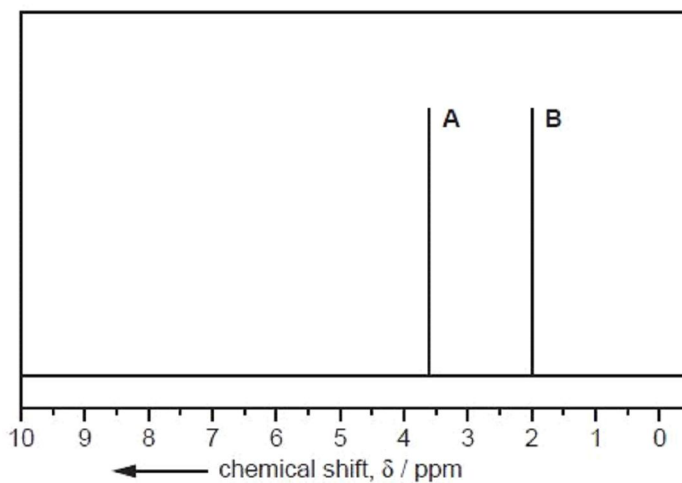
- (a) One instrumental technique is NMR spectroscopy, which uses the fact that under certain conditions protons can exist in two different energy states.
Explain how these different energy states arise.

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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]

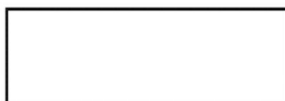
- (c) The NMR spectrum below is that of one of three possible isomers of molecular formula $\text{C}_3\text{H}_6\text{O}_2$.



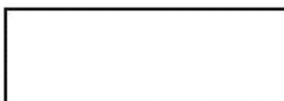
The compound could be propanoic acid, methyl ethanoate or ethyl methanoate.

For
Examiner's
Use

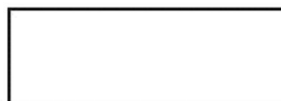
(i) In the boxes provided, draw the structures of the three compounds.



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**.

.....
.....
.....

(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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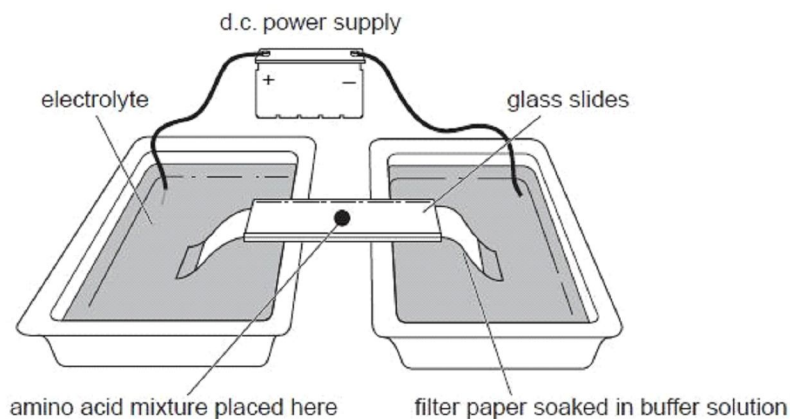
[2]

[Total: 10]

Q5.

- 7 A mixture of amino acids may be separated using electrophoresis. A typical practical set-up is shown in the diagram.

For
Examiner's
Use



- (a) When the power supply is switched on, some amino acids may **not** move, but remain stationary. Suggest an explanation for this observation.

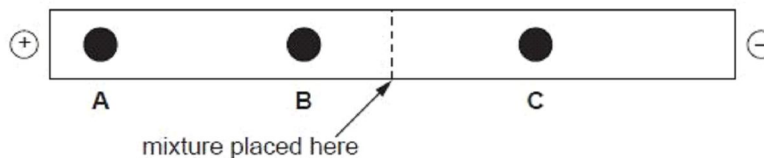
.....

 [2]

- (b) The amino acid glycine has the formula $\text{H}_2\text{NCH}_2\text{CO}_2\text{H}$. Identify the species formed on the filter paper if glycine moves to the left (positive) end of the filter paper.

..... [1]

- (c) The following result was obtained from another electrophoresis. What can be deduced about the relative sizes of, and charges on, the amino acid species **A**, **B** and **C**?



amino acid	relative size	charge
A		
B		
C		

[3]

(d) The sequence of amino acids in a polypeptide may be determined by partial hydrolysis of the chain into smaller pieces, often tripeptides.

(i) Following such a partial hydrolysis, the following tripeptides were obtained from a given polypeptide.

ala-gly-asp gly-ala-gly lys-val-ser ser-ala-gly val-ser-ala

Given that the N-terminal amino acid is lysine (lys) suggest the amino acid sequence of the **shortest** polypeptide that would give the above tripeptides.

.....

The structural formulae of the amino acids in the polypeptide are given below.

abbreviation	amino acid	structural formula
ala	alanine	$\text{H}_2\text{NCH}(\text{CH}_3)\text{CO}_2\text{H}$
asp	aspartic acid	$\text{H}_2\text{NCH}(\text{CH}_2\text{CO}_2\text{H})\text{CO}_2\text{H}$
gly	glycine	$\text{H}_2\text{NCH}_2\text{CO}_2\text{H}$
lys	lysine	$\text{H}_2\text{NCH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2)\text{CO}_2\text{H}$
ser	serine	$\text{H}_2\text{NCH}(\text{CH}_2\text{OH})\text{CO}_2\text{H}$
val	valine	$\text{H}_2\text{NCH}(\text{CH}(\text{CH}_3)_2)\text{CO}_2\text{H}$

(ii) Which of the tripeptides in (i) has the lowest M_r ?

.....

(iii) Select **one** amino acid **from those listed in the table** which contains an ionic side-chain at pH 8.

.....

[4]

[Total: 10]

Q6.

- 8 Chromatography is an important analytical technique in chemistry. There is a number of techniques under the general heading of chromatography.

For
Examiner's
Use

- (a) Paper and gas chromatography rely on partition to separate the components in a mixture, whereas thin-layer chromatography uses adsorption.

Explain what is meant by (i) *partition* and (ii) *adsorption*, in the context of chromatography.

(i) partition

.....

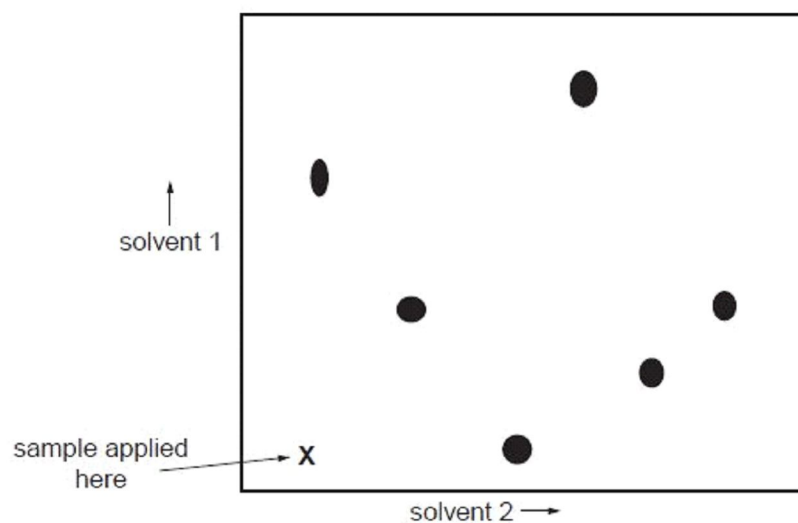
.....

(ii) adsorption

.....

..... [2]

- (b) In paper or thin-layer 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.

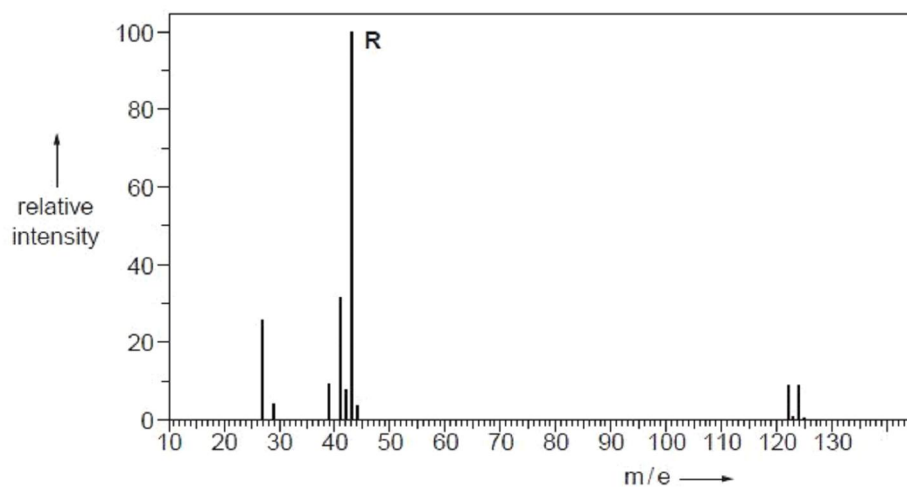


- (i) Ring the spot which was insoluble in solvent 1.
(ii) Label as **A** and **B** the spots which were **not** resolved using solvent 1.

[2]

- (c) The mass spectrum shown was obtained from a compound of formula C_pH_qX , where X represents a halogen atom.

For
Examiner's
Use



- (i) Deduce the identity of X , giving a reason.

X is

.....

- (ii) If the relative heights of the M and $M+1$ peaks are 9 and 0.3 respectively, calculate the value of p . Use this value and the m/e value of the molecular ion to calculate the value of q , and hence the molecular formula of the compound. Show your working.

- (iii) Suggest a formula for the ion responsible for the peak labelled **R**.

..... [4]

- (d) In the fragmentation of alcohols which occurs in a mass spectrometer, small stable, neutral molecules are sometimes produced. Suggest the identity of **two** such molecules, each with an M_r less than 30.

(i) (ii) [2]

[Total: 10]

Q7.

7 The technique of DNA fingerprinting has been one of the most important developments in biochemical analysis in recent times. It has enabled enormous advances to be made in forensic science, medicine and archaeology.

(a) The table shows different stages in the production of a genetic fingerprint. Use the numbers 1 to 6 to put the stages in the correct sequence in the blank column.

stages	process	correct sequence (numbers)
A	place samples on agarose gel	
B	use polymerase chain reaction	
C	label with radioactive isotope	
D	extract DNA	
E	use restriction enzyme	
F	carry out electrophoresis	

[3]

(b) One of the stages above uses a radioactive isotope.

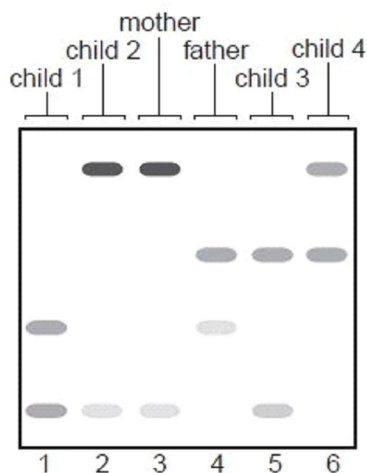
(i) What isotope is used?

(ii) Why is this isotope chosen?

.....

[2]

(c) The following DNA fingerprints were taken from a family of mother, father and four children.



(i) Are all of the children related to the mother? State the evidence for your answer.

For
Examiner's
Use

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.....

(ii) Which child is unlikely to be related to the father? State the evidence for your answer.

.....
.....

[2]

(d) DNA fingerprinting has been successfully used in archaeological investigations.

(i) Ancient writings were often made on goatskins. Over the centuries these have often become broken into fragments, making reconstruction of the writings almost impossible.

Suggest how the use of DNA fingerprinting might be able to identify which fragments came from a particular skin.

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(ii) Apart from the examples of human remains and goatskins, state one other material that could be investigated using this technique.

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[3]

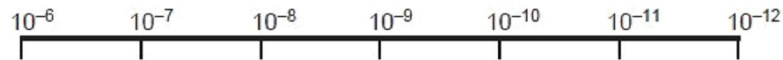
[Total: 10]

Q8.

8 Nanotechnology is a fast-developing area of science based on the ability to manipulate materials of very small dimensions.

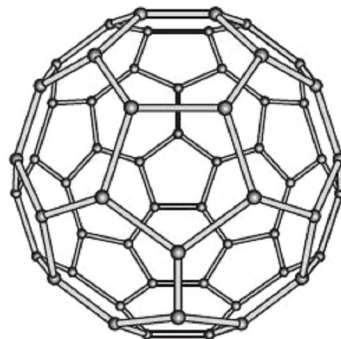
For
Examiner's
Use

(a) On the scale shown in metres, mark the upper and lower limits of the range of sizes for nanoparticles.



[2]

(b) One of the most commonly recognised nanoparticles is the 'buckyball', a spherical form of carbon containing 60 carbon atoms. It has been referred to as the third allotrope of carbon.



Diamond and graphite are two other allotropes of carbon. Suggest what is meant by the term *allotrope*.

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..... [2]

(c) Nanoparticles are used to deliver drugs within cells. Suggest what property of nanoparticles enables them to be used in this way. Explain your answer.

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.....
..... [2]

(d) Copper is an important metal that has been used for thousands of years. The problem today is that most of the ores rich in copper compounds have been used up. A century ago ores containing >2% of copper by mass would have been worked; today's mines have to operate at much lower percentages, down to 0.5% of copper by mass.

(i) By what *type of reaction* is the copper present in the ore converted to copper metal?

.....

One of the main ores of copper contains the mineral *chalcopyrite*, CuFeS_2 .

(ii) Calculate the percentage of copper by mass in *chalcopyrite*.

(iii) If the ore contains 2% of *chalcopyrite* by mass, calculate the mass of copper which can be produced from each tonne of ore.

(iv) Certain bacteria are able to extract copper from the 'spoil' heaps of previously mined copper ore. These bacteria are sprayed onto the spoil heaps in an aqueous solution and the resulting solution containing iron(II) sulfate and copper(II) sulfate is collected in tanks.

Suggest how the copper could be recovered as metal.

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[4]

[Total: 10]

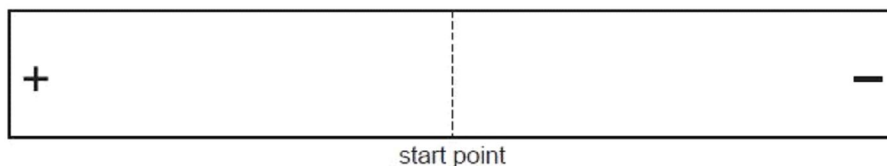
Q9.

7 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	$\text{H}_3\text{N}^+\text{CH}_2\text{CO}_2^-$
lysine	$\text{H}_3\text{N}^+\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_3^+)\text{CO}_2^-$
glutamic acid	$\text{H}_3\text{N}^+\text{CH}(\text{CH}_2\text{CH}_2\text{CO}_2^-)\text{CO}_2^-$

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*.

.....

.....

.....

(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]

Q10.

- 7 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.

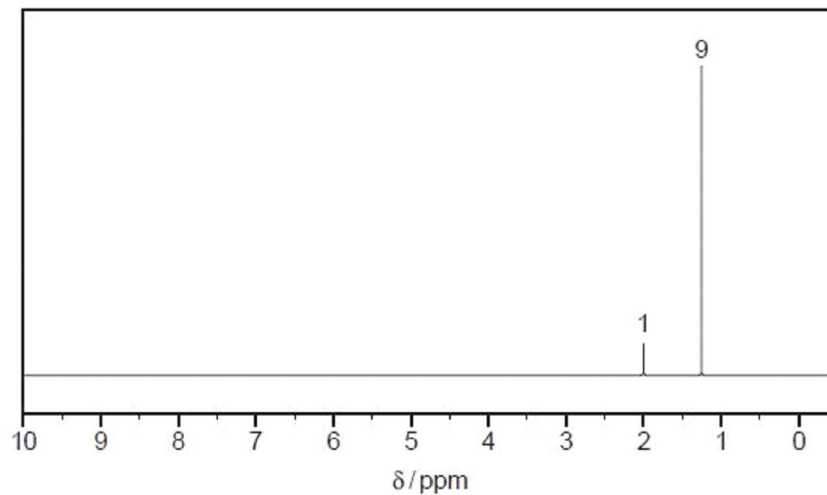
Two factors can influence the energy required for this promotion. What are they?

(i)

(ii)

[2]

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



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

peak at 1.26δ peak at 2.0δ

structure of **J**

- (b) Complete the table by indicating whether the items can be used for DNA fingerprinting. Use a tick (✓) for items which can be used for DNA fingerprinting and a cross (x) for items which cannot.

item for testing	suitable for DNA fingerprinting
human hair	
piece of a flint tool	
piece of Iron Age pot	
piece of Roman leather	

[3]

- (c) Various forms of chromatography can be used to separate and analyse mixtures. HPLC (high performance liquid chromatography) can be used to separate each of the following mixtures. State another method of chromatography which would separate each mixture.

insecticides in a sample of water

dyes present in a foodstuff

drug residue in an athlete's urine

[3]

[Total: 10]

Q12.

7 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.

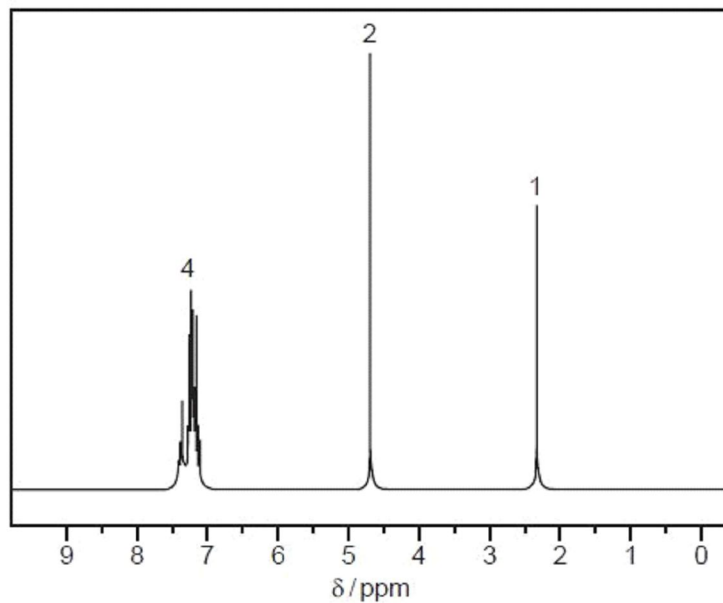
(i) Use the data to calculate the number of carbon atoms present in **L**.

(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.

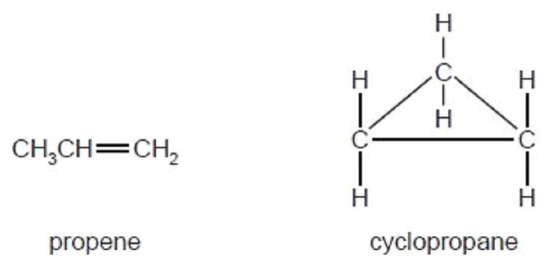
f
Exam
L

structure of **L**



[7]

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

Q13.

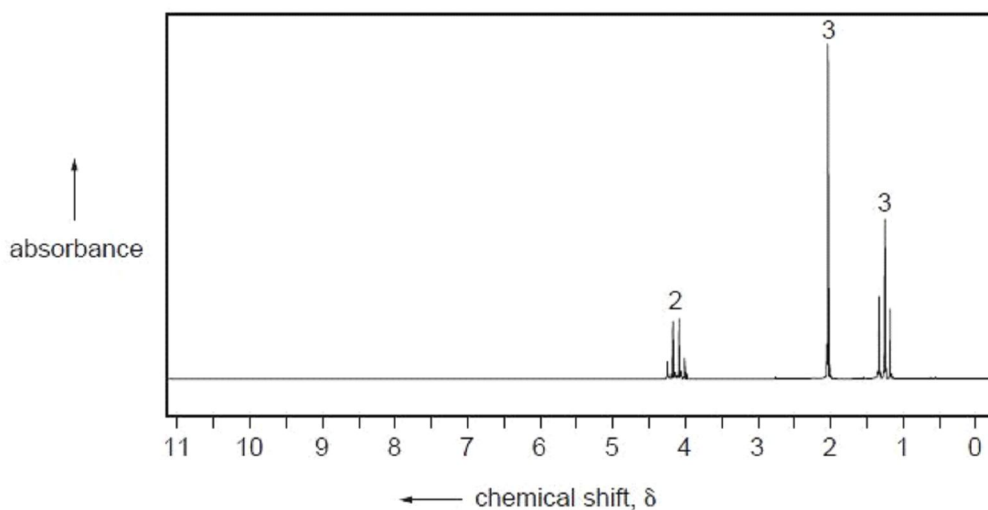
- 9 (a) Explain with reference to energy states how ^1H NMR can supply information about the structure of molecules.

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.....
.....[3]

- (b) Nuclear magnetic resonance is used in magnetic resonance imaging scanners. These scanners are increasingly used in hospitals to detect tumours. Suggest why magnetic resonance techniques are better than X-rays.

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.....[2]

- (c) The NMR spectrum shown below was obtained from a simple organic molecule, **G**, $\text{C}_x\text{H}_y\text{O}_z$. 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**.

[5]

[Total: 10]

Q14.

1 (a) Natural bromine consists of the two isotopes ^{79}Br and ^{81}Br in roughly equal proportions.

The mass spectrum of bromine consists of 5 peaks.

(i) Suggest the mass numbers for the 5 peaks and the identities of the species responsible for them.

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.....

(ii) Suggest the ratios of the relative abundances of

- the three lines with the highest mass numbers,

.....

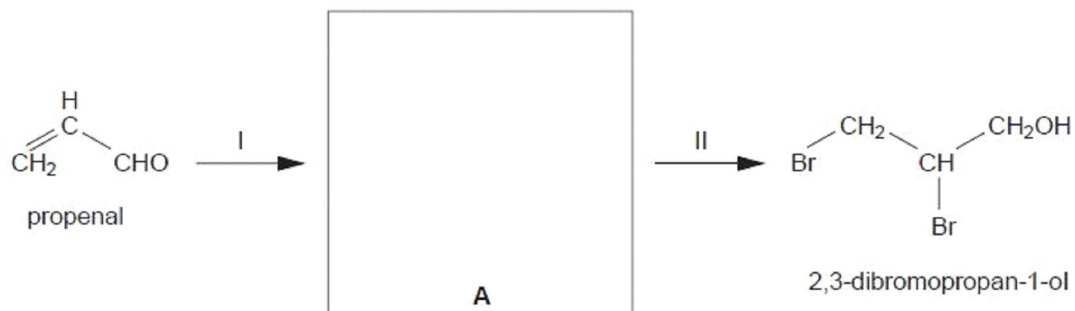
- the two lines with the lowest mass numbers.

.....

[4]

Esters of 2,3-dibromopropan-1-ol with phosphoric acid are useful flame retardants used in plastics and fibres.

2,3-dibromopropan-1-ol can be made from propenal by the following two-stage process.



(b) (i) Draw the structure of the intermediate **A** in the box opposite.

(ii) Suggest reagents and conditions for

- reaction I,

.....

- reaction II.

.....

[3]

(c) The mass spectrum of 2,3-dibromopropan-1-ol includes the following peaks.

mass number	relative abundance
31	100
106	44
108	45
185	0.3
187	0.6
189	0.3

(i) At what mass number would you expect the molecular ion to occur?

.....

(ii) Identify the molecular formula (including isotopic composition where relevant) of these 6 peaks.

mass number	molecular formula
31	
106	
108	
185	
187	
189	

[5]

[Total: 12]

Q15.

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

US

(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?

.....

(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.

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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.

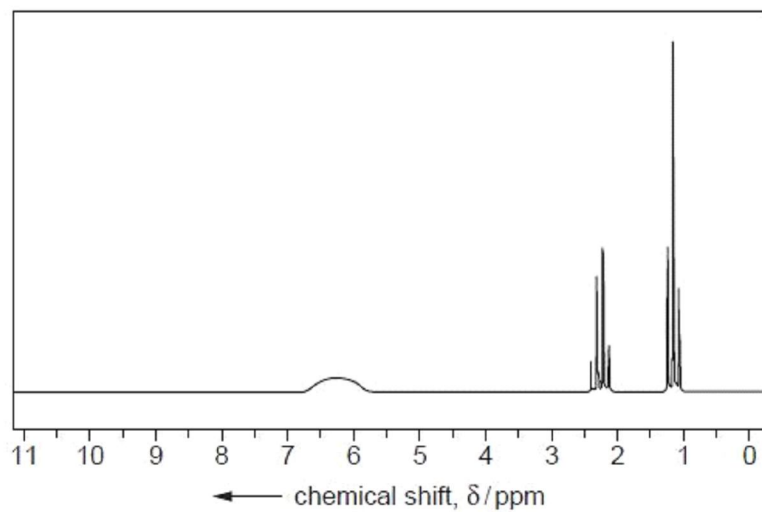
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[3]

(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.



[4]

[Total: 10]

Q16.

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

For
Examiner's
Use

(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.

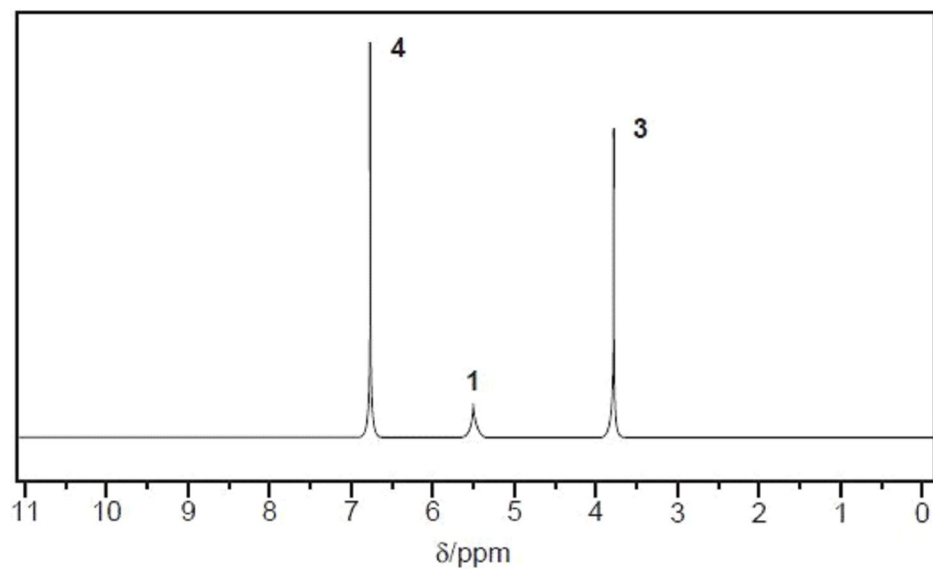
(i) What feature of protons enables their detection by NMR spectroscopy?

.....

- (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.

Exa

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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.....

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.....

.....

Possible structure of **X**

[6]

[Total:10]

Q17.

8 The residues from organohalogen pesticides are known to be a major cause of the decline in numbers of different birds of prey in many countries. These residues are concentrated in birds at the top of food chains.

- (a) Analysis of the bodies of birds of prey show that the pesticide residues accumulate in the fatty tissues of the birds. This is because of the high partition coefficient between the fat in the tissues and water found in blood.

Explain what is meant by the term *partition coefficient*.

.....

 [2]

- (b) A particular pesticide has a partition coefficient of 8.0 between the solvent hexane and water. If a 25 cm³ sample of water containing 0.0050 g of the pesticide is shaken with a 25 cm³ sample of hexane, calculate the mass of pesticide that will dissolve in the hexane layer.

[2]

(c) Compounds used as pesticides may contain bromine or chlorine.

- (i) What would be the difference in the ratio of the M: M+2 peaks if the pesticide contained one chlorine rather than one bromine atom?

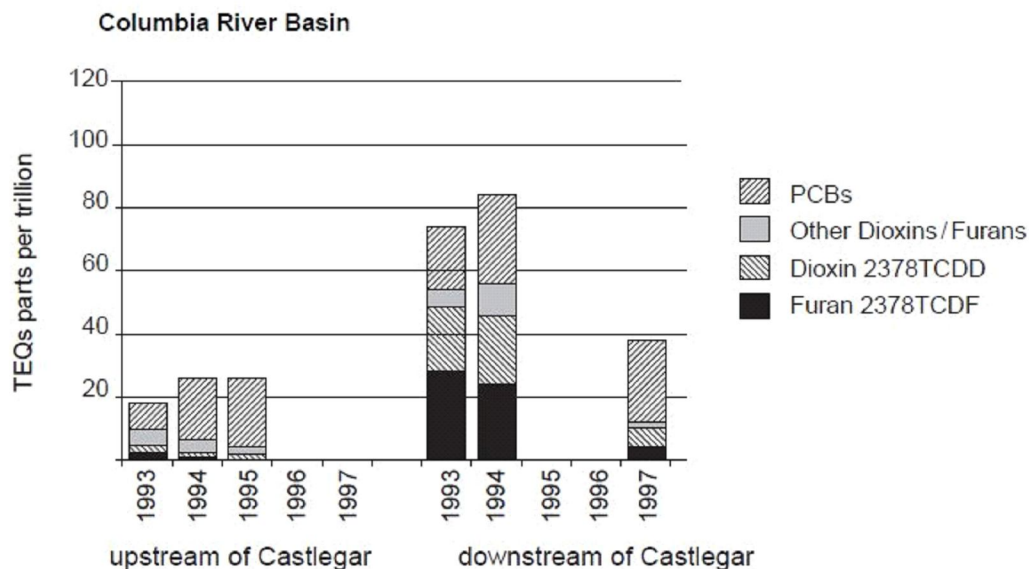
.....

- (ii) If a given pesticide contains **two** chlorine atoms per molecule, deduce the relative heights of the M, M+2 and M+4 peaks.

[3]

- (d) The following graph shows the occurrence of pesticide residues in the eggs of fish-eating birds of prey upstream and downstream of a paper mill at Castlegar on the Columbia River in Canada.

For
Examiner's
Use



PCBs, the dioxin 2378TCDD, and the furan 2378TCDF all come from chemicals containing chlorine.

- (i) Suggest which compounds are present directly as a result of the paper mill.
-
- (ii) By studying the data for 1994, suggest which chemical(s) come from sources other than the paper mill.
-
- (iii) Compare the downstream data for 1994 with that for 1997. Suggest what might be responsible for the change.
-
- (iv) A molecule of 2378TCDD contains four chlorine atoms. How many molecular ion peaks would this compound show in its mass spectrum?
-

[4]

[Total:11]

Q18.

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

For
Examiner's
Use

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

NMR.....

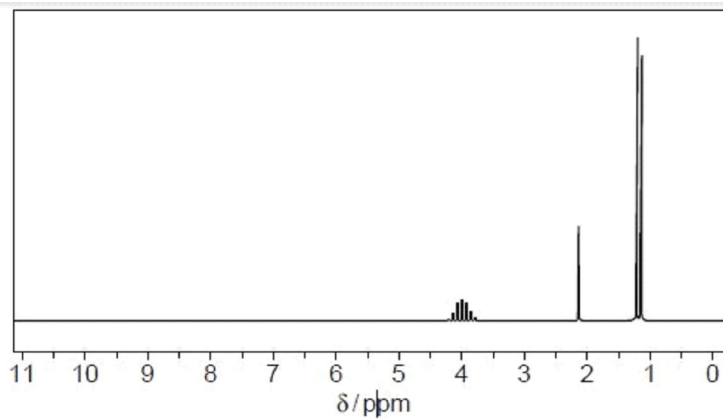
.....

X-ray

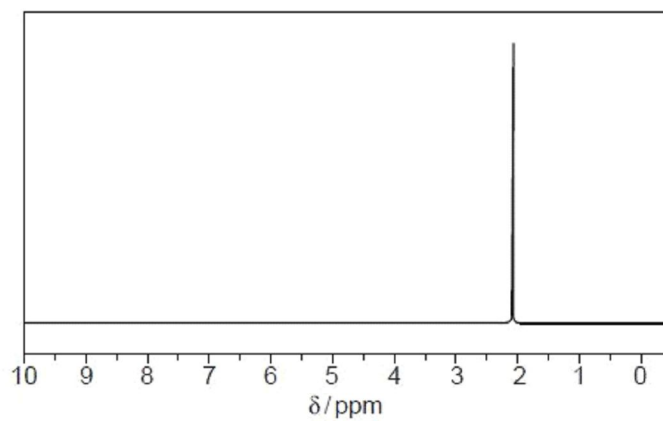
.....

[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



- (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]

Q19.

10 Instrumental methods of analysis have become increasingly important in recent years. The use of chromatography to separate substances, and NMR spectroscopy to identify them, has become routine in many laboratories.

For
Examiner's
Use

(a) Chromatography relies on either partition or adsorption to help separate substances.

(i) Briefly explain how each method brings about separation.

partition

.....

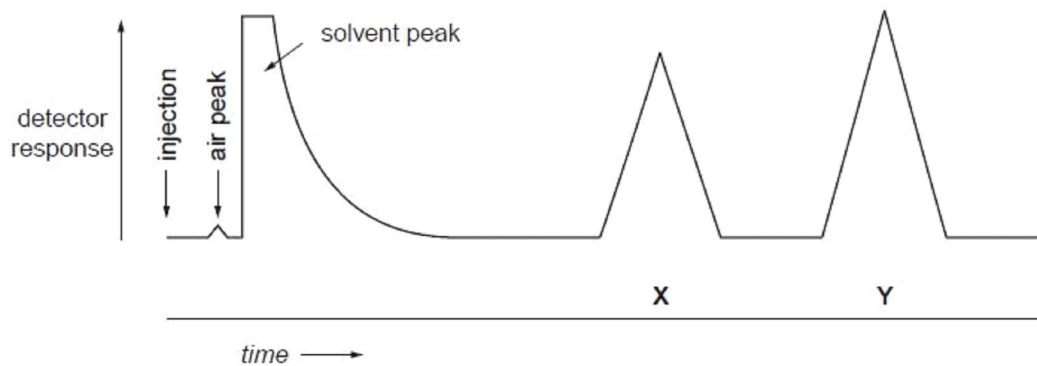
adsorption

.....

(ii) The table shows three different techniques of chromatography. Identify which separation method, *partition or adsorption*, applies to each.

technique	separation method
paper chromatography	
thin-layer chromatography	
gas/liquid chromatography	

(iii) The diagram represents the output from gas/liquid chromatography carried out on a mixture.



Determine the percentage of each of the two components **X** and **Y** in the mixture.

[5]

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

For
Examiner's
Use

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

.....
.....

(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.

.....
.....
.....
.....

[4]

[Total: 9]

Q20.

7 One of the key areas of investigation in understanding the structures of polypeptides and proteins is the sequence of amino acids that make up the polypeptide chains.

For
Examiner's
Use

(a) One of the methods used to determine the amino acids present in a polypeptide chain is electrophoresis.

Sketch and label the apparatus used to carry out electrophoresis.

[4]

(b) In electrophoresis, different amino acids move in different directions and at different speeds.

(i) What factors determine the *direction of travel* of an amino acid?

.....
.....
.....

(ii) What factors determine the *speed of movement* of an amino acid?

.....
.....

[3]

(c) Another important technique used to examine the structure of proteins is X-ray crystallography. In this technique the position of individual atoms can be determined, and the distances between them measured.

For
Examiner's
Use

(i) Hydrogen atoms never produce images using X-ray crystallography. Explain why this is the case.

.....
.....

(ii) Suggest and explain which one of the atoms in a molecule of cysteine, $\text{H}_2\text{NCH}(\text{CH}_2\text{SH})\text{CO}_2\text{H}$, would show up most clearly using X-ray crystallography.

.....
.....

[3]

[Total: 10]

Q21.

- 7 Different analytical techniques are used to build up a picture of complex molecules. Each technique on its own provides different information about complex molecules but together the techniques can give valuable structural information.

For
Examiner's
Use

- (a) Complete the table, identifying the technique which can provide the appropriate structural information.

structural information	analytical technique
three-dimensional arrangement of atoms and bonds in a molecule	
chemical environment of protons in a molecule	
identity of amino acids present in a polypeptide	

[3]

- (b) One general method of separating organic molecules is chromatography. Briefly explain the chemical principles involved in each of the following techniques.

- (i) paper chromatography

.....

.....

.....

- (ii) thin-layer chromatography

.....

.....

.....

[2]

- (c) A combination of mass spectrometry and NMR spectroscopy is often enough to determine the structure of a simple organic compound.

For
Examiner's
Use

The organic compound **N** produced a mass spectrum in which the ratio of the M:M+1 peaks was 5.9:0.20, and which had an M+2 peak of similar height to the M peak.

- (i) Calculate how many carbon atoms are present in one molecule of **N**.

- (ii) Deduce which element, other than carbon and hydrogen, is present in **N**.

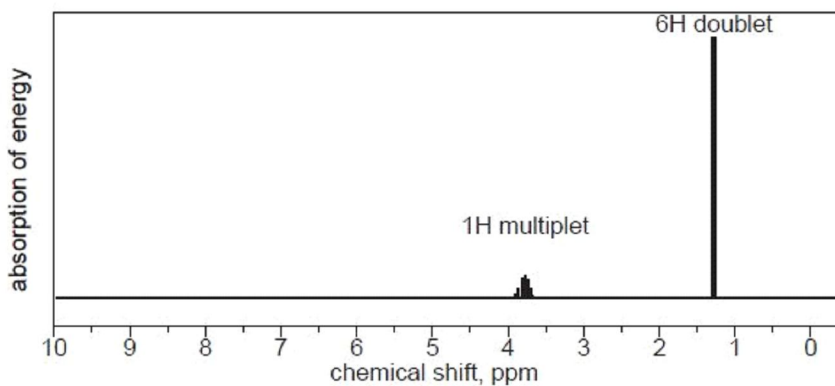
.....

- (iii) Explain how many atoms of this element are present in one molecule of **N**.

.....

.....

The NMR spectrum of **N** is shown.



- (iv) State the empirical formula of **N** and, using the NMR data, suggest the structural formula of **N**, explaining your reasons.

[6]

[Total: 11]

Q22.

7 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) (i) 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?

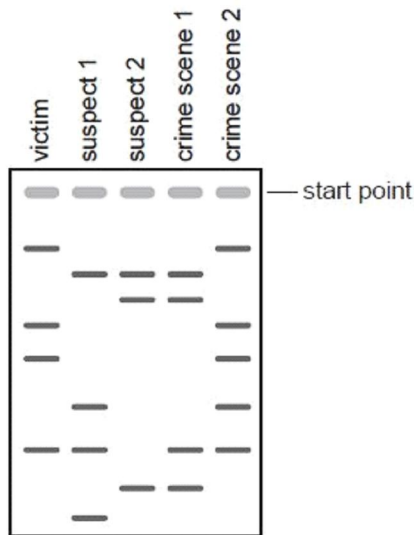
.....

(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.

.....

.....

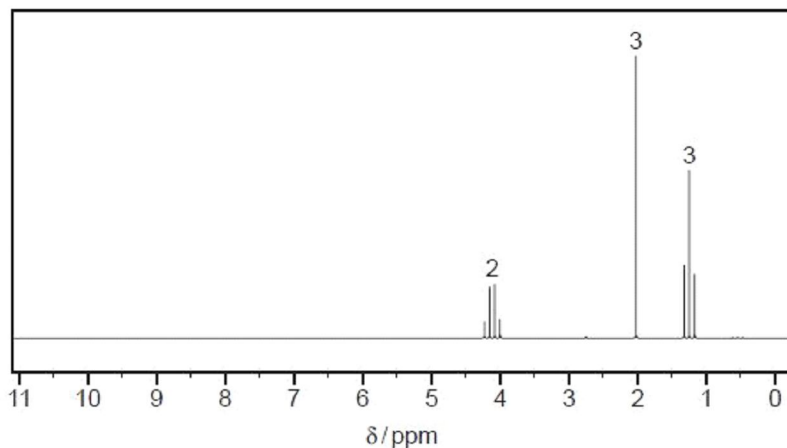
[2]

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

For
Examiner's
Use

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.

.....

.....

.....

.....

.....

.....

.....

.....

structure of **P**

[5]

[Total: 10]

Q23.

- 7 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.

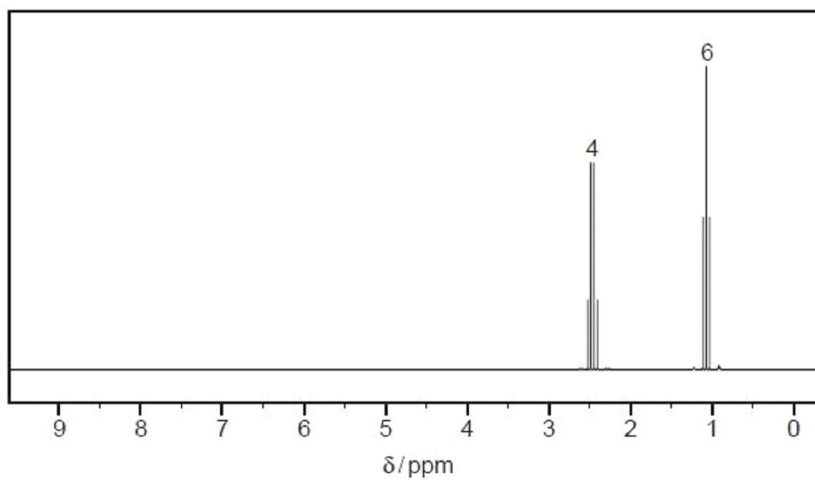
For
Examiner:
Use

- (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]

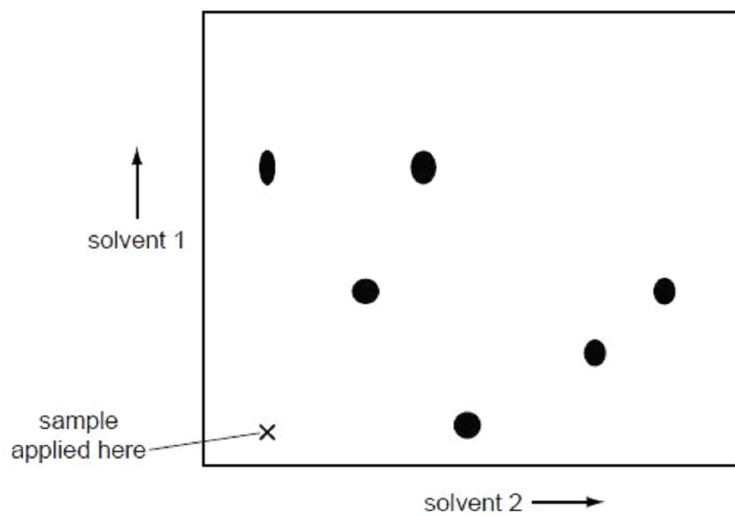
(b) Chromatography is another important analytical technique used in chemistry.

(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.

Fc
Exami
Us



(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]

Q24.

7 Electrophoresis is a technique which can be used to separate amino acids or peptide fragments present in a mixture. Ex

(a) Draw a diagram to show the apparatus used to carry out electrophoresis. You should label each of the relevant parts of the apparatus.

[4]

(b) How far an amino acid will travel during electrophoresis depends on the pH of the solution. For a given potential difference, state **two other** factors that will affect how far a given amino acid travels in a fixed time during electrophoresis.

1.

.....

2.

.....

[2]

(c) A number of analytical and separation techniques rely on substances having different partition coefficients.

State what is meant by the term *partition coefficient*.

.....

.....

.....

[1]

- (d) The partition coefficient of **X** between ethoxyethane and water is 40.0.
A solution contains 4.00 g of **X** dissolved in 0.500 dm³ of water.

F
Exam
U

Calculate the mass of **X** that can be extracted from this aqueous solution by shaking it with

- (i) 0.050 dm³ of ethoxyethane,
- (ii) two successive portions of 0.025 dm³ of ethoxyethane.

[4]

[Total: 11]

Q25.

8 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]

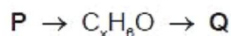
- (b) NMR spectroscopy provides detailed information about protons, but X-ray crystallography is unable to detect them. Explain these facts.

.....
.....
.....
.....
[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]

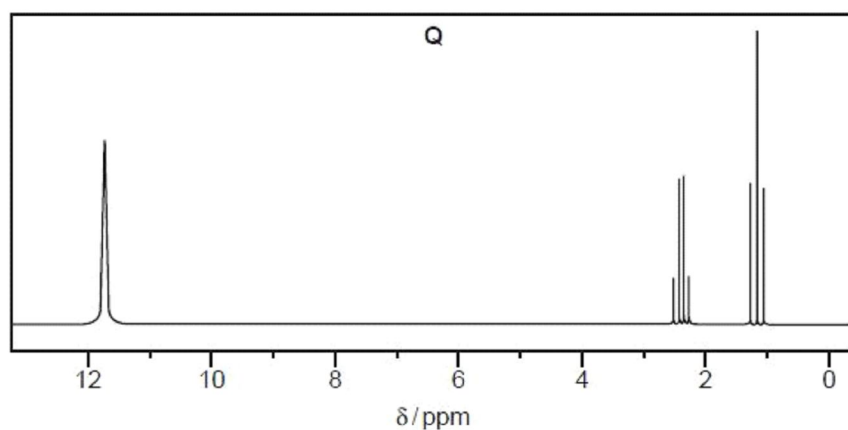
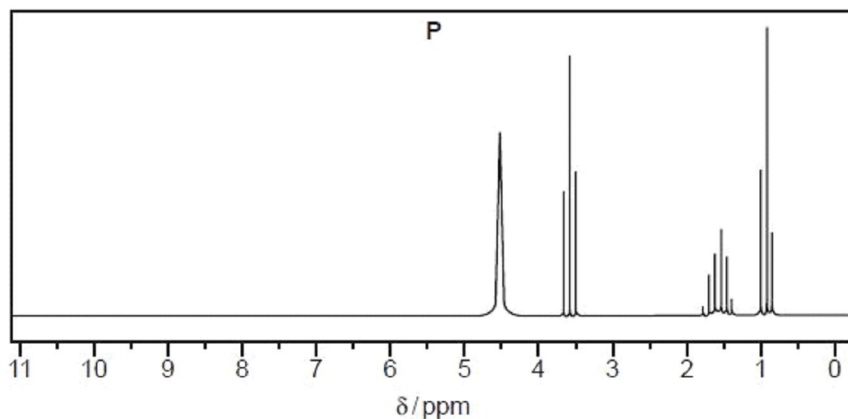
- (d) Compound **P** is an alcohol that can be converted into compound **Q** in the following reaction sequence.



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

[6]

[Total: 10]

