

Name:

Date:

NMR

Past paper questions booklet International A Level Chemistry

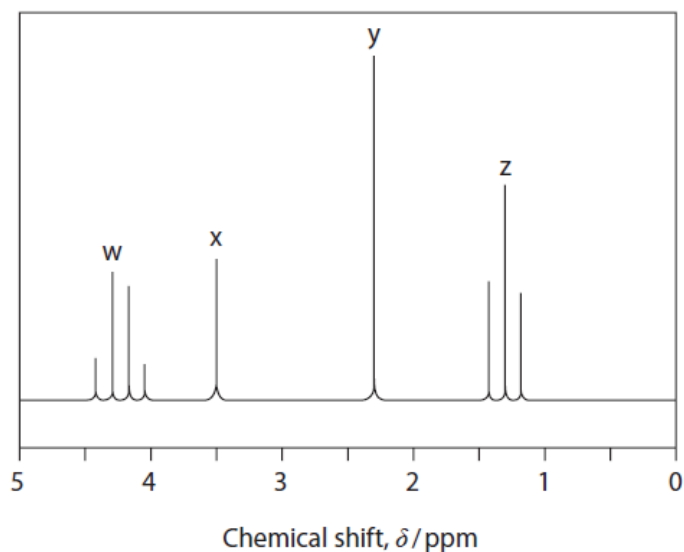
SECTION B

Answer ALL the questions.

Write your answers in the spaces provided.

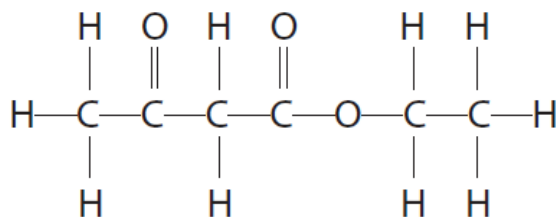
16 The compound ethyl 3-oxobutanoate, which is used in food flavouring, has the formula $\text{CH}_3\text{COCH}_2\text{COOCH}_2\text{CH}_3$.

The high resolution proton (^1H) NMR spectrum of this compound is



(a) (i) Identify which groups of hydrogen atoms are responsible for each peak in the spectrum by adding the labels w, x, y and z to the appropriate parts of this displayed formula to match the letters on the spectrum.

(2)



(ii) Explain the splitting patterns of the peaks at 4.2 ppm and 1.3 ppm.

(2)

(iii) The carbon-13 (^{13}C) NMR spectrum of ethyl 3-oxobutanoate has six peaks.

Draw the structure of an **isomer** of ethyl 3-oxobutanoate that contains a carboxylic acid group and a ketone functional group, but only has four peaks in its carbon-13 NMR spectrum.

(1)

17 This question concerns six isomers each with the molecular formula $C_5H_{10}O_2$.

(a) Isomers **A**, **B**, **C** and **D** are structural isomers that all react with aqueous sodium carbonate to produce carbon dioxide.

Isomer **A** is a straight-chain compound.

Isomer **B** has only two peaks in its high resolution proton NMR spectrum, both of which are singlets.

Isomer **C** contains a chiral centre but isomer **D** does not.

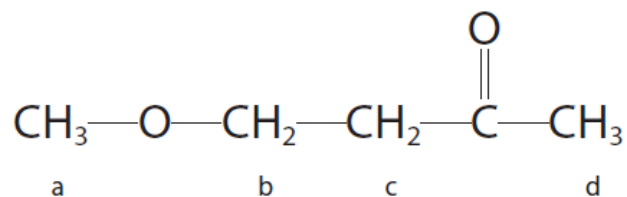
Give the structures of these **four** isomers.

(4)

A	B

C	D

- (b) (i) Isomer **E** contains an ether functional group (R-O-R) and a ketone functional group. The **low** resolution proton NMR spectrum of isomer **E** has four peaks. The displayed formula of isomer **E** is



The four hydrogen environments responsible for the four peaks are labelled. Complete the table of information regarding these peaks including the splitting pattern in the **high** resolution spectrum.

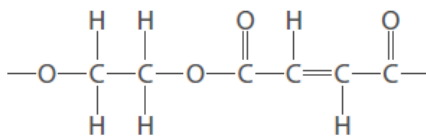
(3)

Peak	a	b	c	d
Relative peak area	3			
Chemical shift range, δ / ppm	2.9 – 4.2			
Splitting	singlet			

- (ii) State the number of peaks in the carbon-13 (^{13}C) NMR spectrum of **E**.

(1)

(c) The repeat unit of a polyester is shown.



Give the structures of the two monomers that could form this polyester.

(2)

Monomer 1	Monomer 2

(d) An organic compound **E** contains carbon, hydrogen and oxygen only.

(i) The accurate relative atomic masses, A_r , of the three elements in **E** are shown in the table.

Element	A_r
hydrogen	1.0078
carbon	12.0000
oxygen	15.9949

E contains five carbon atoms and gives a molecular ion peak at $m/z = 102.0678$ in its mass spectrum.

Deduce the molecular formula of **E**.

(1)

- (ii) Aqueous sodium hydrogencarbonate is added to a sample of **E**.
No effervescence occurs.

State what can be deduced by this observation.

(1)

- (iii) The infrared spectrum of **E** has an absorption in the range $1750 - 1735 \text{ cm}^{-1}$.

Name the functional group in **E**.

(1)

- (iv) Data from the high resolution proton NMR spectrum of **E** is shown.

Peak	Chemical shift, δ / ppm for TMS	Splitting pattern	Relative peak area
A	4.02	triplet	2
B	2.05	singlet	3
C	1.65	sextet	2
D	0.95	triplet	3

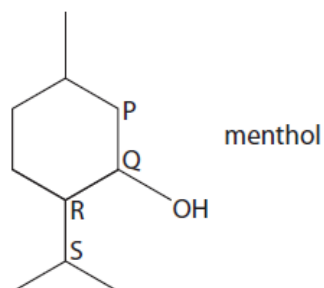
Deduce the structure of **E**.

Justify your answer by labelling the protons responsible for each peak.

(3)

(Total for Question 17 = 14 marks)

- 8 The compound menthol has the structure shown.
Some of the carbon atoms are labelled P, Q, R and S.



- (a) What is the number of chiral centres in a molecule of menthol?

(1)

- A 1
- B 2
- C 3
- D 4

- (b) Which of the carbon atoms is responsible for a peak at 72 ppm in the ^{13}C NMR spectrum of menthol?

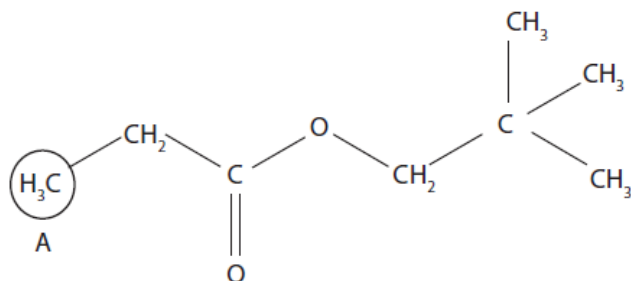
(1)

- A P
- B Q
- C R
- D S

(c) The high resolution proton NMR spectrum of compound Y was obtained.

(i) Label the three remaining hydrogen environments B, C and D on the structure.

(1)



(ii) Complete the table.

(3)

Hydrogen environment	Splitting pattern of peak	Relative peak area
A	triplet	3
B		
C		
D		

(Total for Question 17 = 9 marks)

SECTION B

Answer ALL the questions. Write your answers in the spaces provided.

16 Compound **X** is used by mammals as an alternative energy source to sugars.
X is a compound of carbon, hydrogen and oxygen only.

(a) Complete combustion of a 2.50 g sample of **X** in dry oxygen produced
4.31 g of carbon dioxide and 1.32 g of water as the only products.

(i) Give a reason why the oxygen used must be dry.

(1)

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(ii) Show that the empirical formula of **X** is $C_4H_6O_3$. You **must** show your working.

(5)

(b) Compound **X** gave an orange precipitate with Brady's reagent (2,4-dinitrophenylhydrazine) but no reaction with Tollens' reagent. When **X** was added to a solution of sodium hydrogencarbonate, effervescence occurred and the gas evolved turned limewater cloudy.

The carbon-13 NMR spectrum of **X** had only four peaks.

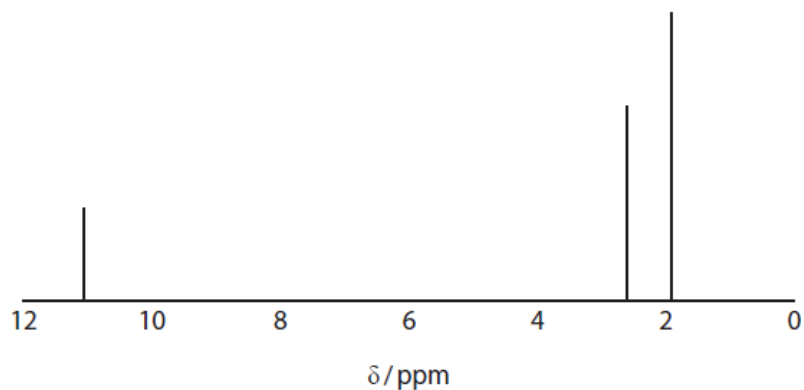
(i) Deduce the **two** possible structures of **X**, showing how this information supports your answer.

(6)

(ii) Give a **chemical** test which would allow you to distinguish between the two compounds you have given in (b)(i). Include the reagents required and the result for each of the compounds.

(3)

(c) A simplified **high** resolution proton (^1H) NMR spectrum of compound **X** is shown.



Explain how the number of peaks in the ^1H NMR spectrum, together with their relative heights, their chemical shifts and their splitting patterns, may be used to confirm the structure of **X**. Use the chemical shifts given in your Data Booklet.

(5)

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(Total for Question 16 = 20 marks)

(c) Compound **B**, another isomer with the molecular formula $C_6H_{12}O_2$, contains a ring of six carbon atoms.

The carbon-13 NMR spectrum has only two peaks, one of which is at 69 ppm.

Draw the structure of compound **B**.

(2)

(Total for Question 20 = 20 marks)