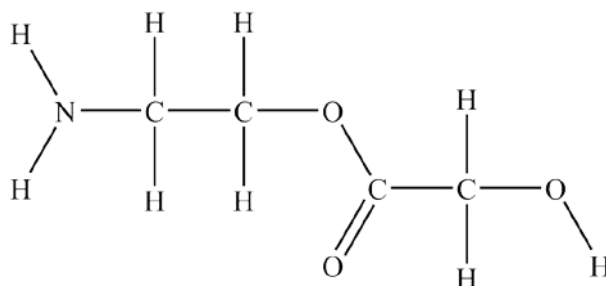


1. The structure of molecule **Z** is shown below.



Which of the following statements is/are true?

- 1: The carbon-13 NMR spectrum of **Z** shows four peaks
- 2: The proton NMR spectrum of **Z** shows five peaks
- 3: The proton NMR spectrum of **Z** run in D₂O shows three peaks

- A 1, 2 and 3
B Only 1 and 2
C Only 2 and 3
D Only 1

Your answer

[1]

2. A chemist isolates compound **L**, with empirical formula C_3H_6O , and sends a sample for analysis. The analytical laboratory sends back the following spectra.

Mass spectrum

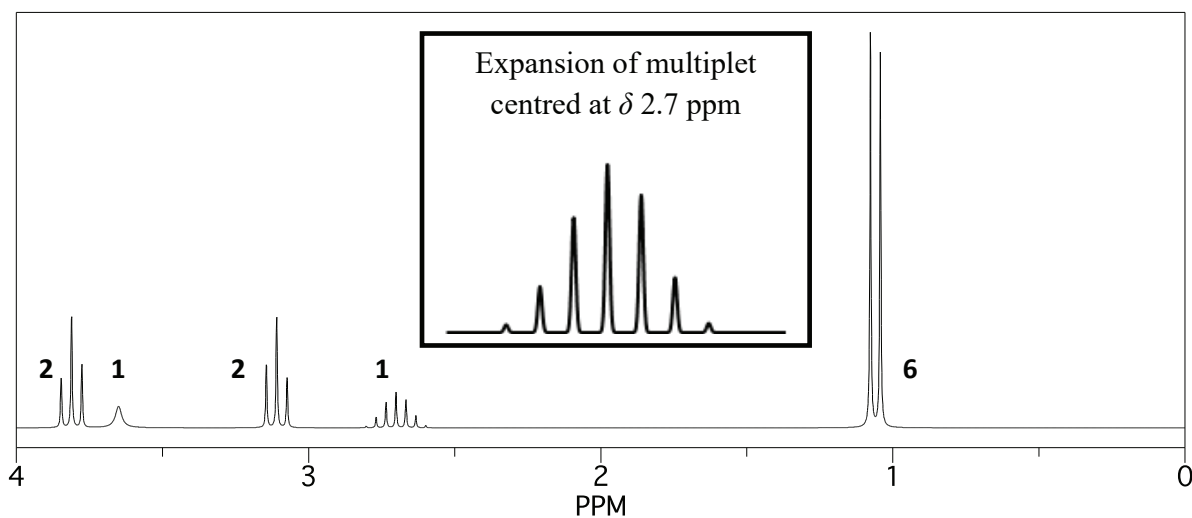
Molecular ion peak at $m/z = 116.0$.

1H NMR spectra

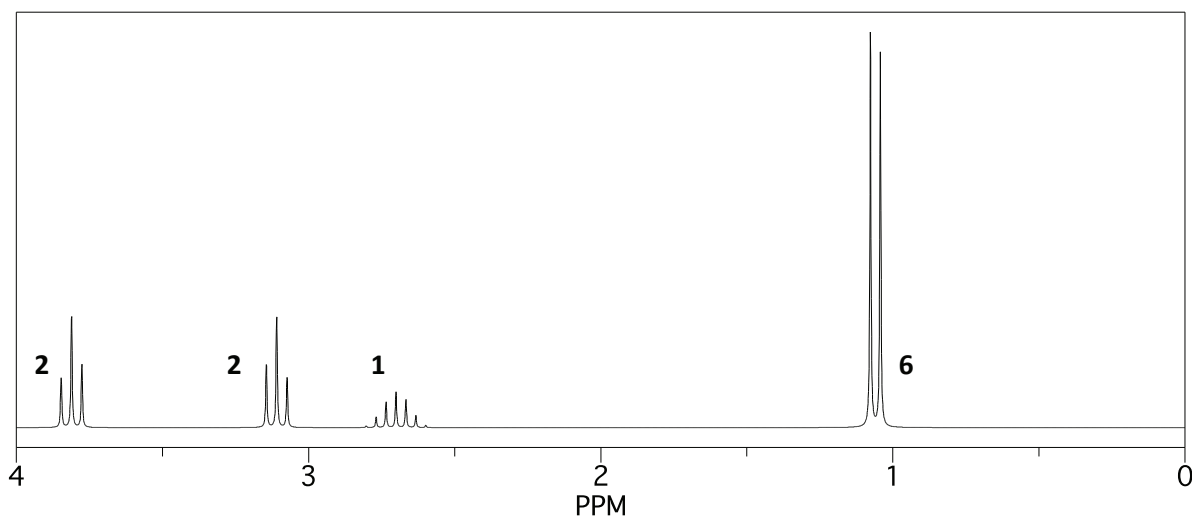
The numbers next to each signal represent the number of 1H responsible for that signal.

Two 1H NMR spectra were obtained: one without D_2O and one with D_2O added.

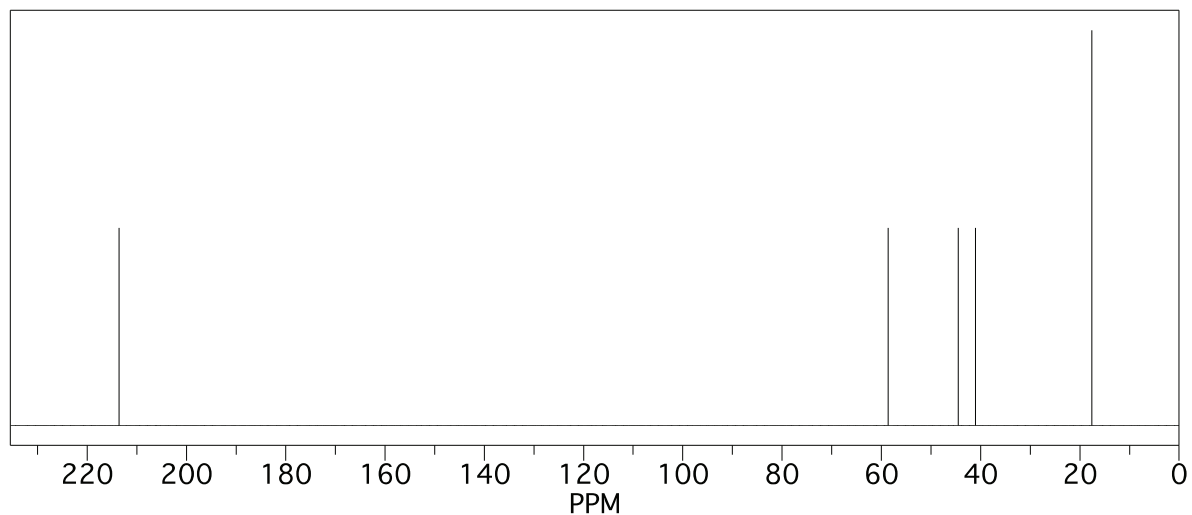
1H NMR spectrum with no D_2O :



1H NMR spectrum with D_2O added:



^{13}C NMR spectrum:



Use the information provided to suggest a structure for compound **L**.

Give your reasoning.

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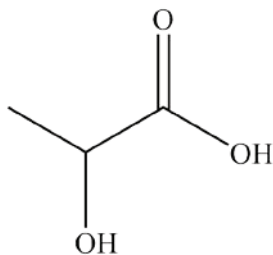
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[6]

3. This question is about organic acids.

(a) Lactic acid, shown below, has two functional groups.



Lactic acid reacts with bases and with many metals.

- An aqueous solution containing 1.125 g of lactic acid is reacted with an excess of magnesium producing hydrogen gas.
- The excess magnesium is removed. The water is evaporated, leaving a white solid, A.

(i) Name the type of reaction of lactic acid with bases and with metals.

reaction with bases:

reaction with metals:

[1]

(ii) Calculate the volume of $\text{H}_2(\text{g})$ produced, measured at room temperature and pressure.

volume of $\text{H}_2 = \dots\dots\dots$ [2]

(iii) What is the empirical formula of the white solid A?

..... [1]

(iv) Predict **two** reactions of lactic acid, each involving a different functional group.

Do **not** include reactions with bases or metals.

For each reaction,

- state the type of reaction, the reagents and conditions
- draw the structures of any organic products formed.

[4]

- (b) In basic conditions, α -amino acids form anions with the general formula, $\text{RCH}(\text{NH}_2)\text{COO}^-$. These anions can act as bidentate ligands.

Copper(II) ions can form a square planar complex with anions of the amino acid glycine ($\text{R} = \text{H}$). There are two stereoisomers of this complex, **B** and **C**.

- (i) Draw the **skeletal** formula of the anion of glycine.

[1]

- (ii) Draw diagrams of stereoisomers **B** and **C**.

In your structures, show the ligands as skeletal formulae.

[2]

- (iii) Anion ligands of the amino acid alanine ($\text{R} = \text{CH}_3$) would be expected to form more than two square planar stereoisomers with copper(II) ions.

Explain this statement.

.....

.....

[1]

- (c) Methanoic acid is added to water. An acid–base equilibrium is set up containing two acid–base pairs.

Suggest a mechanism for the forward reaction in this equilibrium.

Your mechanism should use displayed formulae and curly arrows, and show all species present at equilibrium.

[2]

(d) Information about a monobasic organic acid **D** is shown below.

- **D** reacts by both electrophilic substitution and electrophilic addition.
- The molecular formula of **D** is $C_xH_yO_2$.
- The mass spectrum of **D** has a molecular ion peak at $m/z = 148$.
- The ^{13}C NMR spectrum of **D** contains seven peaks.

Determine and draw a possible structure for **D**.

Explain your reasoning from the evidence provided.

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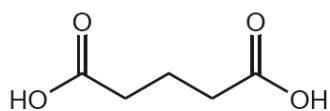
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..... [5]

4. The compound below is analysed by ^1H NMR spectroscopy.



How many peaks are observed in the ^1H NMR spectrum?

- A 5
- B 4
- C 3
- D 2

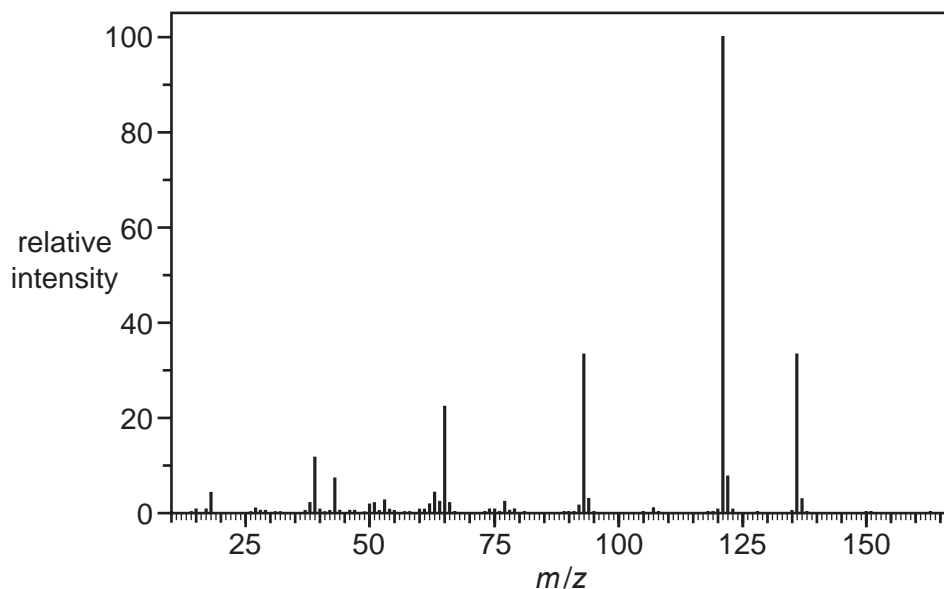
Your answer

[1]

5. A chemist analyses a naturally occurring aromatic compound.
- (a) The percentage composition and mass spectrum of the compound are shown below.

Percentage composition by mass: C, 70.58%; H, 5.92%; O, 23.50%.

Mass spectrum



Determine the molecular formula of the compound.

Show your working.

molecular formula = [3]

- (b) Qualitative tests are carried out on the aromatic compound. The results are shown below.

Test	Acidity	Na ₂ CO ₃ (aq)	2,4-DNP	Tollens' reagent
Observation	pH = 5	No observable change	Orange precipitate	No observable change

Determine the functional groups in the compound. Explain your reasoning.

Functional groups

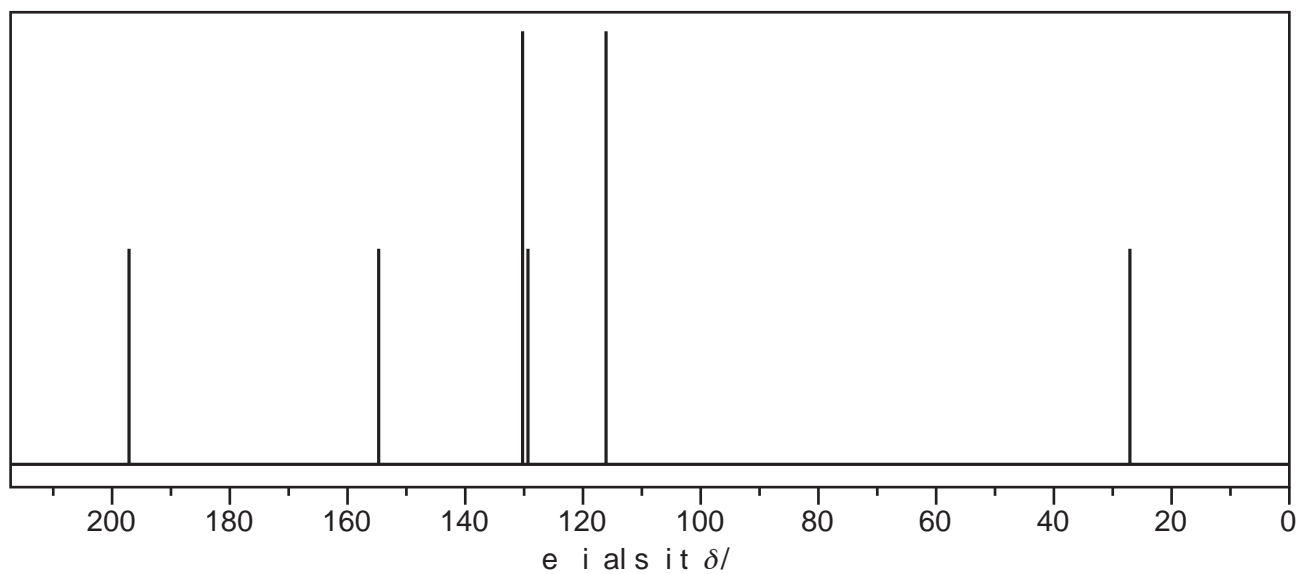
Explanation

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..... [3]

(c) The carbon-13 NMR spectrum of the compound is shown below.



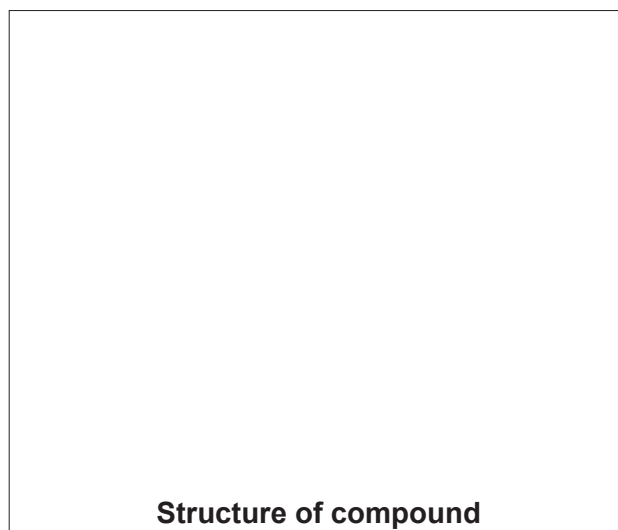
Using the spectrum and the results from (a) and (b), determine the structure of the compound. Explain your reasoning.

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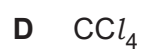
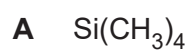
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[3]

6. Which compound is used as a standard for NMR chemical shift measurements?



Your answer

[1]

7. What is the number of peaks in the ^1H NMR spectrum of $\text{HOOCCH}_2\text{CHOHCH}_2\text{COOH}$?

A 3

B 4

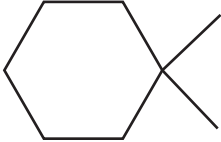
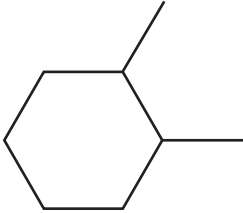
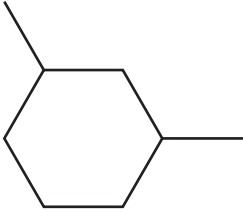
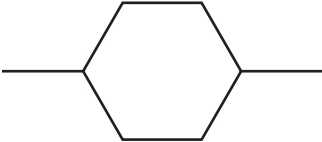
C 5

D 6

Your answer

[1]

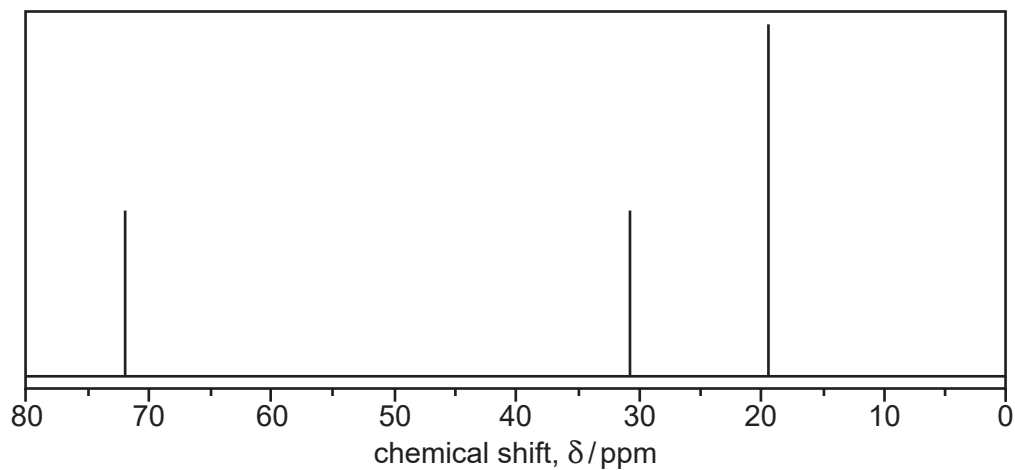
8. Which compound shows 4 peaks in its carbon-13 NMR spectrum?

A	
B	
C	
D	

Your answer

[1]

9. A compound produces the ^{13}C NMR spectrum below.



Which compound could have produced this spectrum?

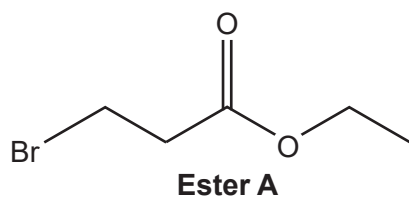
- A Propane
- B 2-Methylbutane
- C 2-Methylpropan-1-ol
- D 2-Methylpropan-2-ol

Your answer

[1]

10. This question is about esters.

(a) The structure of ester **A** is shown below.

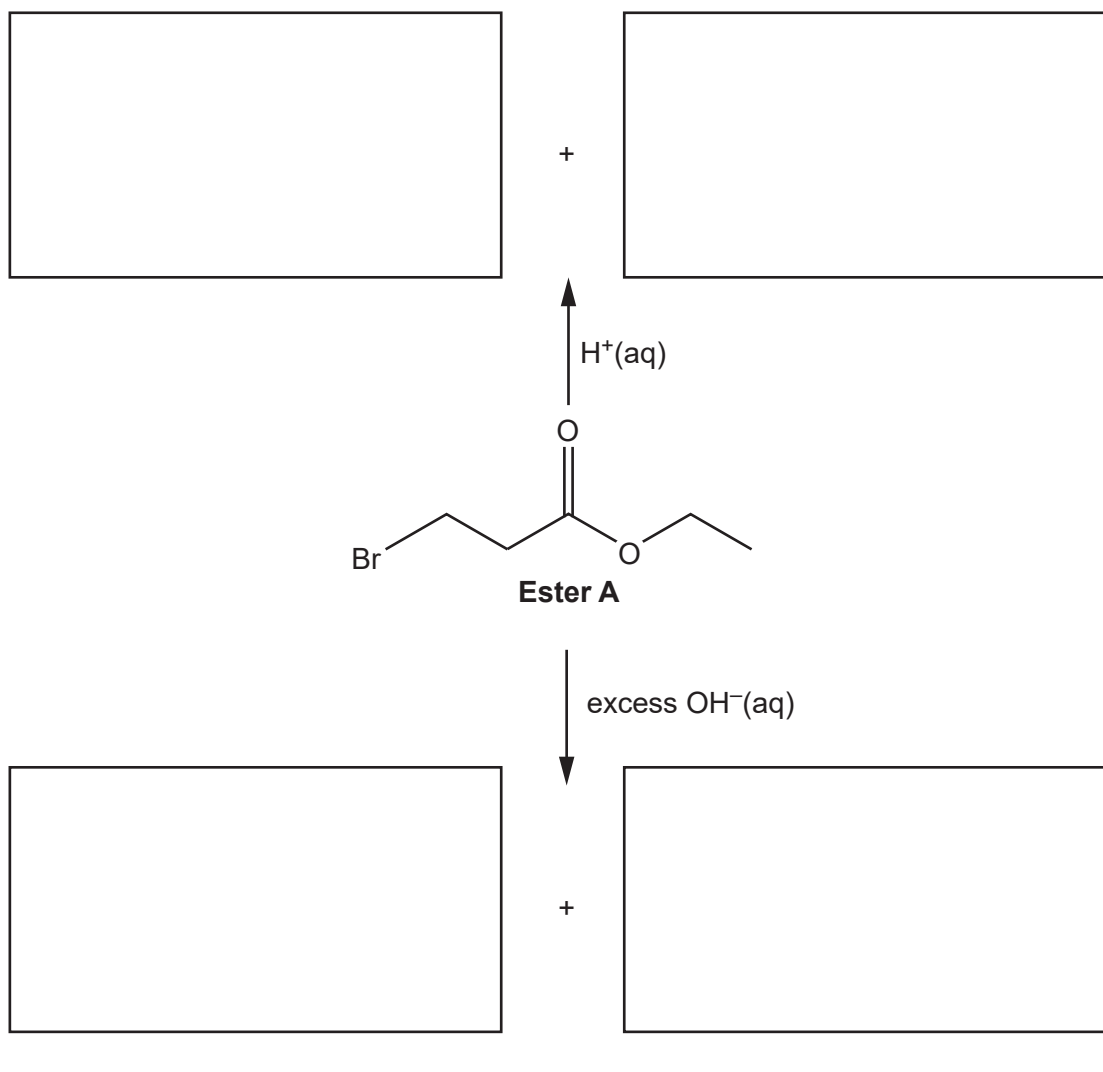


(i) What is the systematic name of ester **A**?

..... [1]

(ii) In the boxes, draw the organic products for the reactions of the functional groups in ester **A** shown below.

Each reaction forms two organic products.

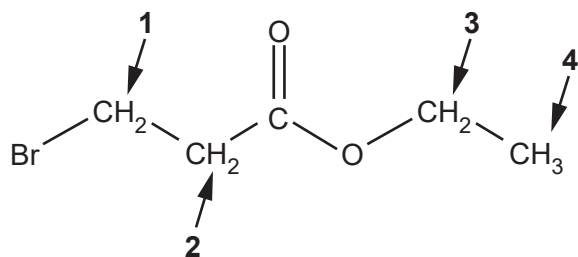


[5]

(iii) Name the type of reactions of ester **A** shown in (ii).

..... [1]

(b) The protons in ester **A** are in four different environments, labelled 1–4 on the structure below.



Complete the table to predict the **proton** NMR spectrum of ester **A**.

Proton environment	Chemical shift	Splitting pattern
1		
2		
3		
4		

[4]

(c) Compound **B** is a structural isomer of ester **A**.

- Compound **B** reacts with aqueous sodium carbonate.
- The ^{13}C NMR spectrum of **B** has 4 peaks.

Draw a possible structure for compound **B**.

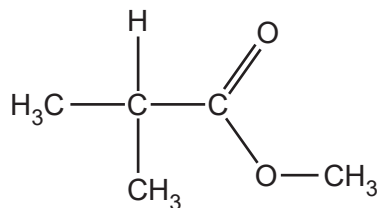
[1]

(d) A polyester is formed from 200 molecules of 4-hydroxybenzoic acid.

What is the relative molecular mass, M_r , of the polyester?

$$M_r = \dots\dots\dots \text{ g mol}^{-1} \text{ [2]}$$

(e)* A student intends to synthesise ester **C**.



Ester C

- (i) Plan a two-stage synthesis to prepare 12.75 g of ester **C** starting from 2-methylpropanal, (CH₃)₂CHCHO. Assume the overall percentage yield of ester **C** from 2-methylpropanal is 40%.

In your answer include the mass of 2-methylpropanal required, reagents, conditions and equations where appropriate.

Purification details are **not** required.

[6]

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Additional answer space if required

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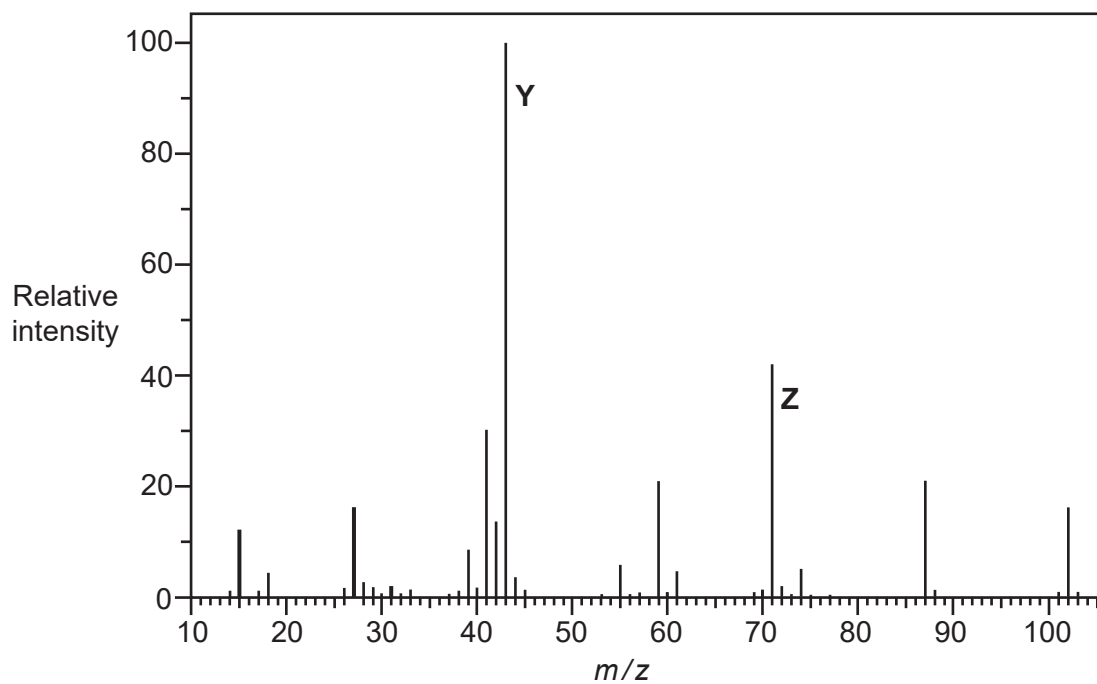
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(ii) The mass spectrum of ester **C** is shown below.



Suggest possible structures for the species responsible for peaks **Y** and **Z** in the mass spectrum.

Y	Z

[2]

11. Analysis of an unknown organic compound produced the following results.

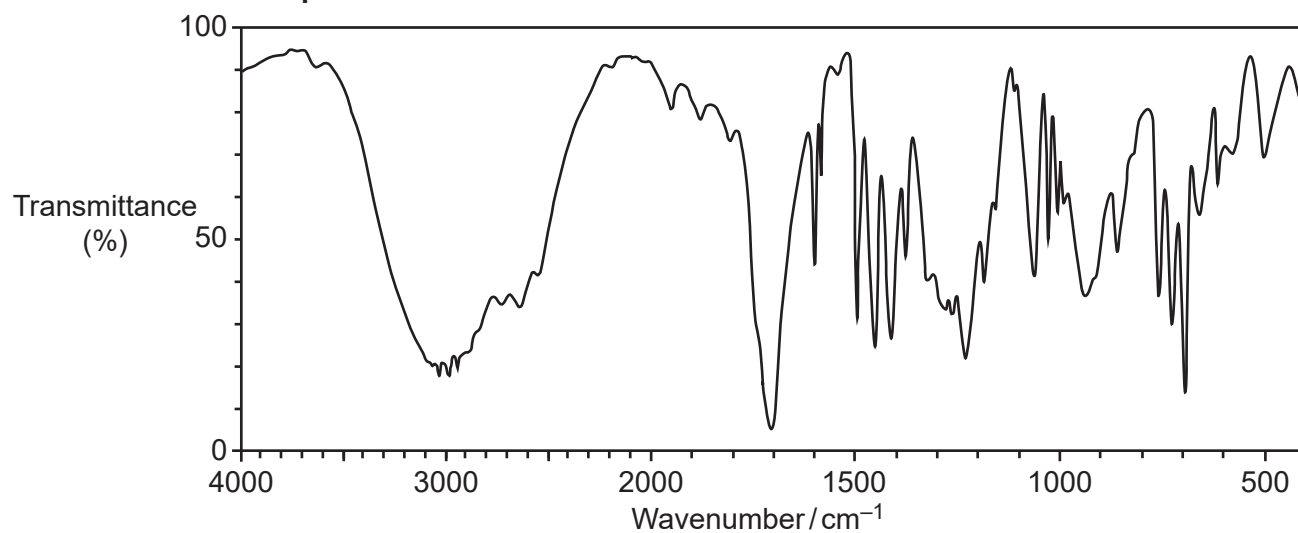
Elemental analysis by mass

C: 73.17%; H: 7.32%; O: 19.51%

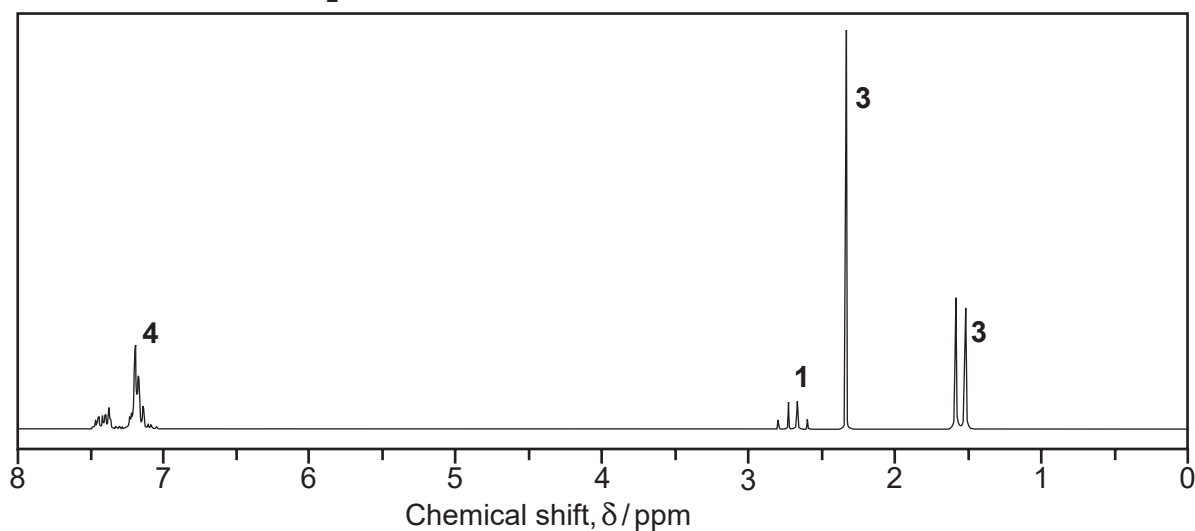
Mass spectrum

Molecular ion peak at $m/z = 164.0$

Infrared spectrum



^1H NMR spectrum in D_2O



The numbers by the peaks are the relative peak areas.

Use the results to suggest **one** possible structure for the unknown compound.

Show **all** your reasoning.

[6]

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Additional answer space if required

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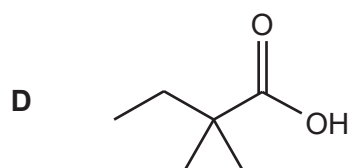
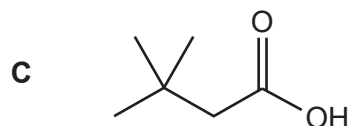
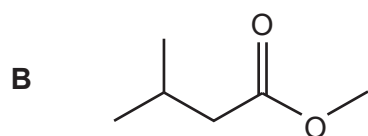
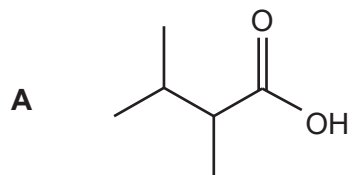
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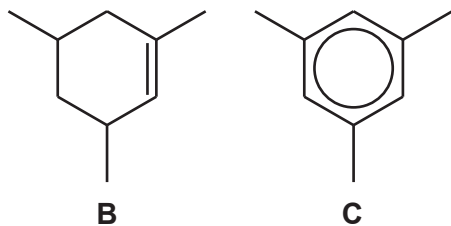
12. Which isomer of $C_6H_{12}O_2$ produces the smallest number of peaks in its ^{13}C NMR spectrum?



Your answer

[1]

13. Compounds **B** and **C**, shown below, are unsaturated hydrocarbons containing nine carbon atoms.



- (a) Compound **B** reacts with chlorine at room temperature, but compound **C** requires the presence of a halogen carrier.

In both reactions, the organic compound reacts with chlorine in a 1:1 molar ratio.

- (i) Draw the structures of the organic product of each reaction.

Organic product with B	Organic product with C

[2]

- (ii) Explain the relative resistance to chlorination of compound **C** compared with compound **B**.

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[3]

(iii) Outline the mechanism for the reaction of compound **C** with chlorine.

Show the role of the halogen carrier.

[5]

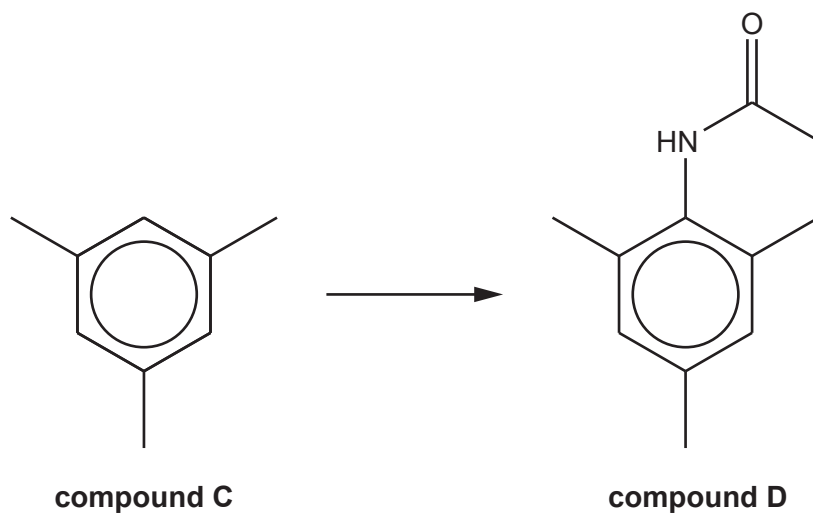
(b) Compound **C** can be prepared by 'trimerisation' of propanone using concentrated sulfuric acid as a catalyst.

Suggest an equation for this reaction, using **molecular** formulae.

..... [3]

(c) An organic chemist is investigating compound **D** for possible use as a medicine.

The chemist proposes a synthesis of compound **D** from compound **C**.



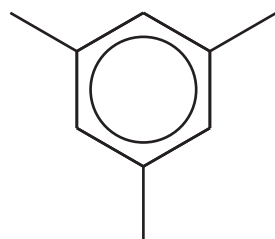
(i) Predict the number of peaks in the ^{13}C NMR spectra of compounds **C** and **D**.

	Compound C	Compound D
Number of peaks

[2]

(ii) The chemist develops a three-stage synthesis of compound **D** from compound **C**.

Complete the flowchart.
Show structures for organic compounds.

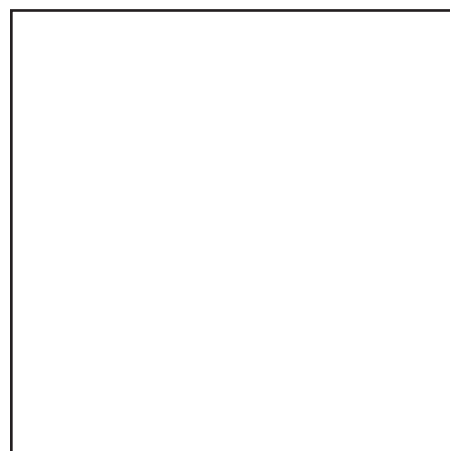


compound **C**

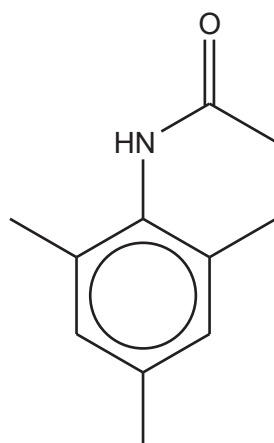
reagent:



catalyst:

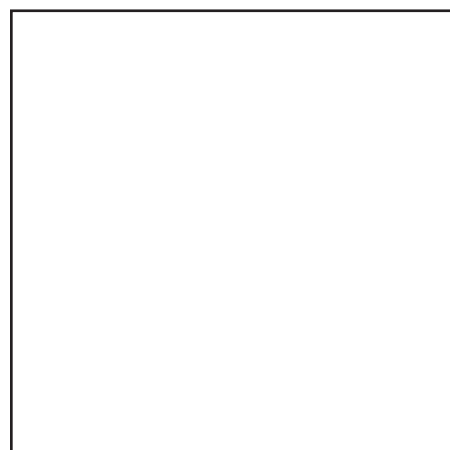


1. Sn + HCl
2. Neutralise



compound **D**

reagent:

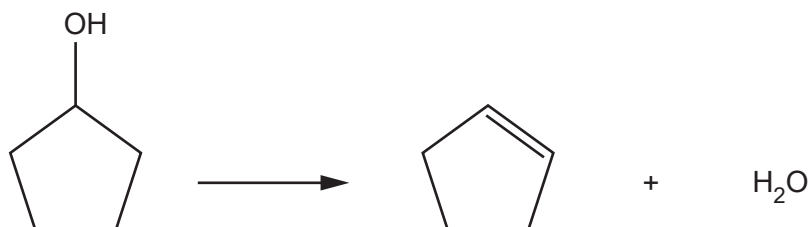


[5]

14. Cyclopentanol can be reacted to form cyclopentene.
Cyclopentene is a liquid with a boiling point of $44\text{ }^{\circ}\text{C}$ and a density of 0.74 g cm^{-3} .

A student plans to prepare 4.00 g of cyclopentene by reacting cyclopentanol (boiling point $140\text{ }^{\circ}\text{C}$) with an acid catalyst.

Equation

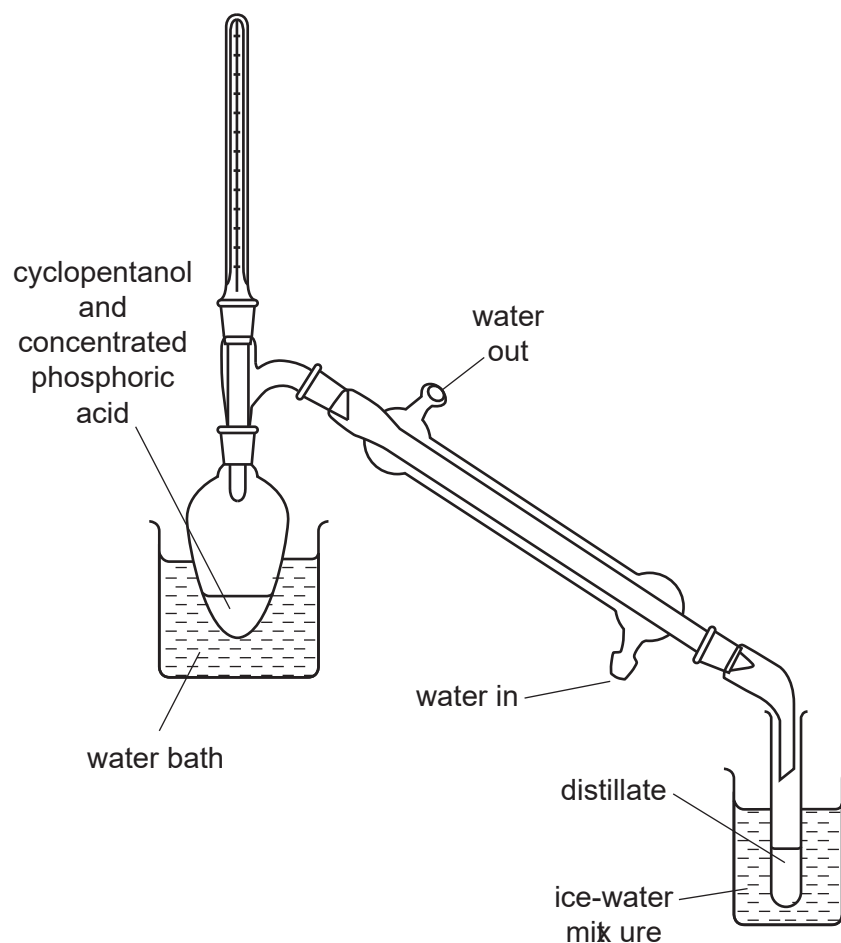


The expected percentage yield of cyclopentene is 64.0% .

Method

The student carries out the preparation using apparatus set up for distillation, as shown below.

- 1 The reaction mixture is heated gently, and a distillate containing impure cyclopentene is collected.



- 2 The distillate has an aqueous layer and an organic layer.
The student purifies the cyclopentene from the distillate.

- (a)* Calculate the mass of cyclopentanol that the student should use and explain how pure cyclopentene could be obtained from the distillate. [6]

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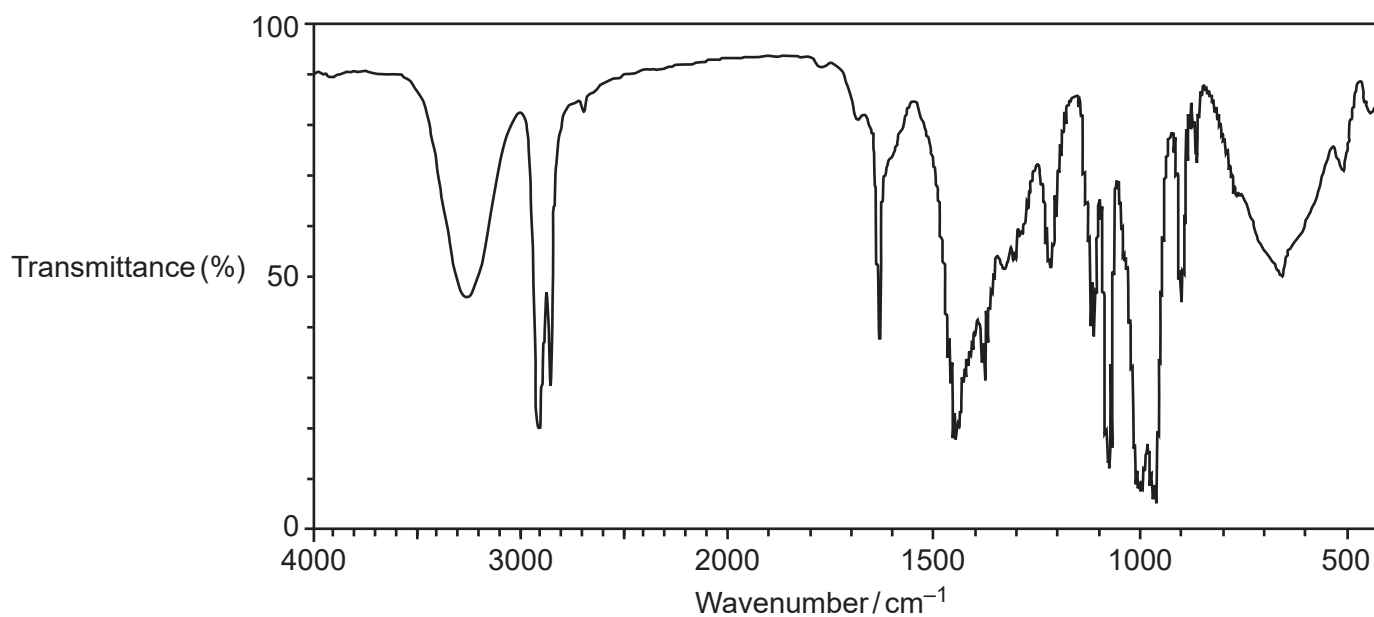
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- (b) The organic layer in the distillate was analysed by IR spectroscopy. The IR spectrum is shown below.



Explain how the IR spectrum of the organic layer suggests that cyclopentene has been formed and that the reaction is incomplete.

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..... [2]

15. An organic compound **I** is analysed, using a combination of techniques. The analytical data is shown below.

Elemental analysis by mass

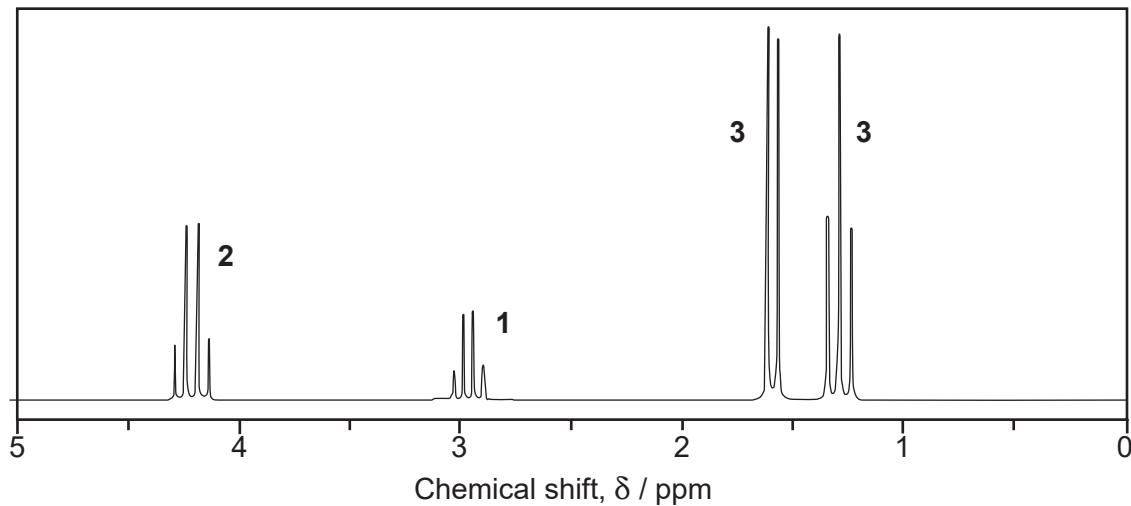
C, 56.69%; H, 7.09%; N, 11.02%; O, 25.20%

Mass spectrum

Molecular ion peak at $m/z = 127.0$

IR spectrum

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Proton NMR spectrum

- (a) Explain the use of two deuterated compounds in NMR spectroscopy.

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..... [2]

(b)* Determine the structure of compound **I**, showing **all** your reasoning.

[6]

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