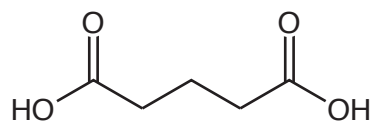


- 1 The compound below is analysed by  $^1\text{H}$  NMR spectroscopy.



How many peaks are observed in the  $^1\text{H}$  NMR spectrum?

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

Your answer

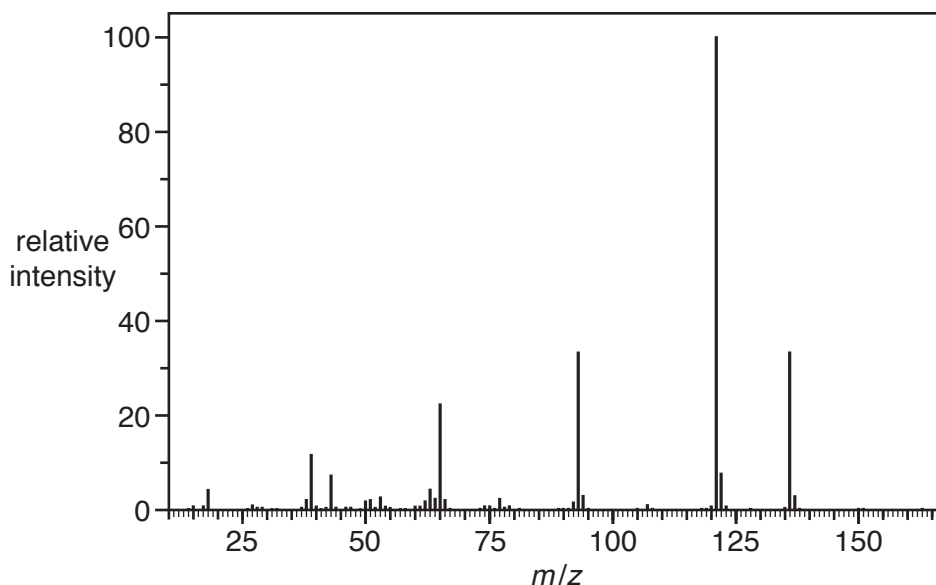
[1]

2 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 | $\text{Na}_2\text{CO}_3(\text{aq})$ | 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 .....

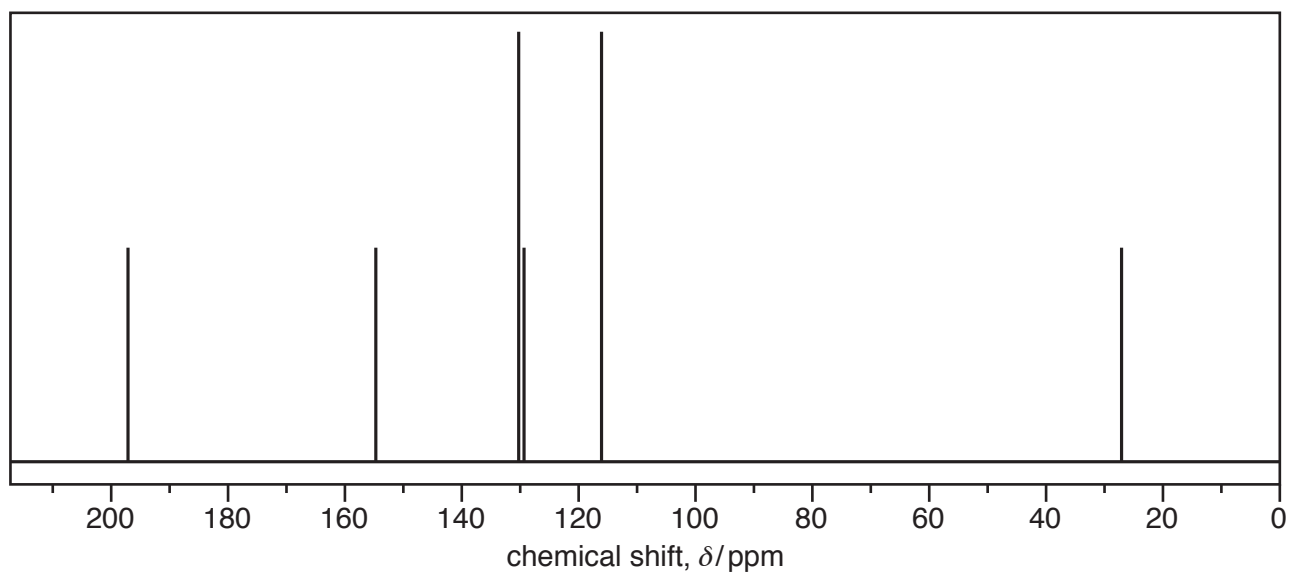
Explanation .....

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..... [3]

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



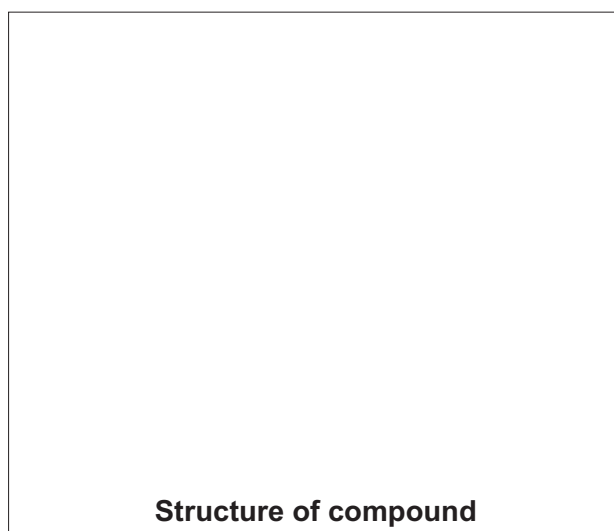
Using the spectrum and the results from (a) and (b), determine the structure of the compound. Explain your reasoning.

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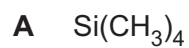
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[3]

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



Your answer

[1]

- 4 What is the number of peaks in the  $^1\text{H}$  NMR spectrum of  $\text{HOOCCH}_2\text{CHOHCH}_2\text{COOH}$ ?
- A** 3
- B** 4
- C** 5
- D** 6

Your answer

[1]

5 A student carries out the nitration of phenol with dilute nitric acid to produce 2-nitrophenol and 4-nitrophenol.

Diagram illustrating the chemical structures of three isomers of nitrophenol:

- 2-nitrophenol**: A benzene ring with a hydroxyl group ( $\text{OH}$ ) at position 1 and a nitro group ( $\text{NO}_2$ ) at position 2.
- 3-nitrophenol**: A benzene ring with a hydroxyl group ( $\text{OH}$ ) at position 1 and a nitro group ( $\text{NO}_2$ ) at position 3.
- 4-nitrophenol**: A benzene ring with a hydroxyl group ( $\text{OH}$ ) at position 1 and a nitro group ( $\text{NO}_2$ ) at position 4.

Explain whether the student is correct.

[3]

- 6\* A scientist is researching compounds that might be suitable as fuel additives. One of the compounds gives the analytical results below.

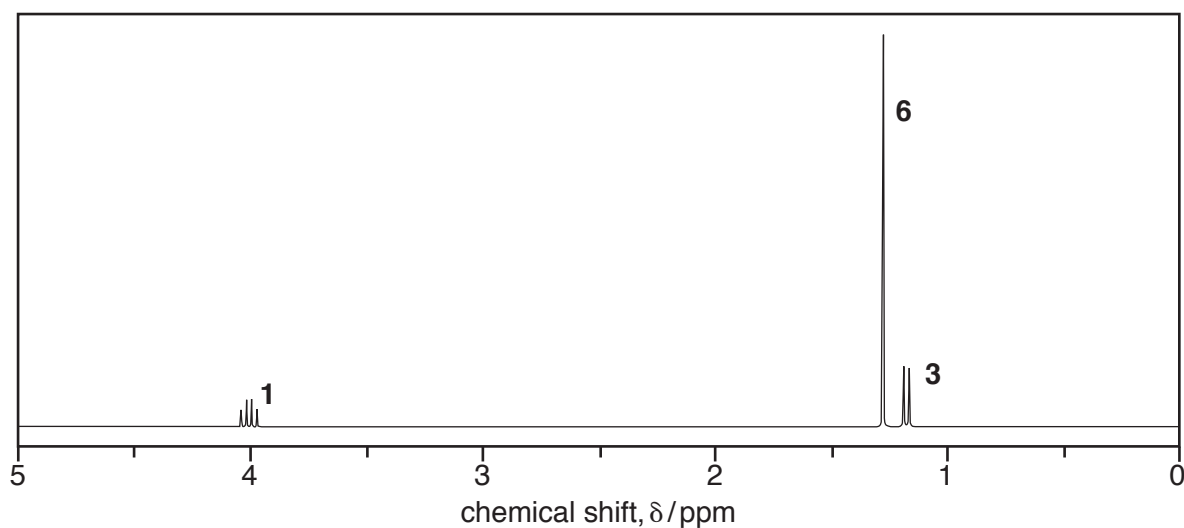
**Elemental analysis by mass:**

C: 54.54%; H: 9.10%; O: 36.36%

**Mass spectrum:**

Molecular ion peak at  $m/z = 132.0$

**$^1\text{H}$  NMR spectrum in  $\text{D}_2\text{O}$**



The numbers by the peaks are the relative peak areas.

When the spectrum is run without  $\text{D}_2\text{O}$ , there are **two** additional peaks with the same relative peak areas at 11.0 ppm and 3.6 ppm.

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

Show **all** your reasoning.

**[6]**

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Additional answer space if required.

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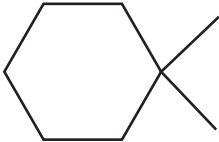
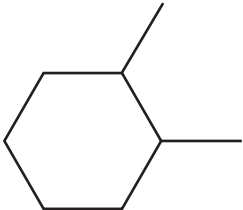
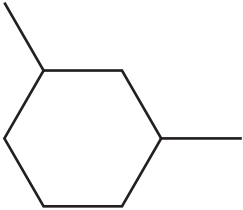
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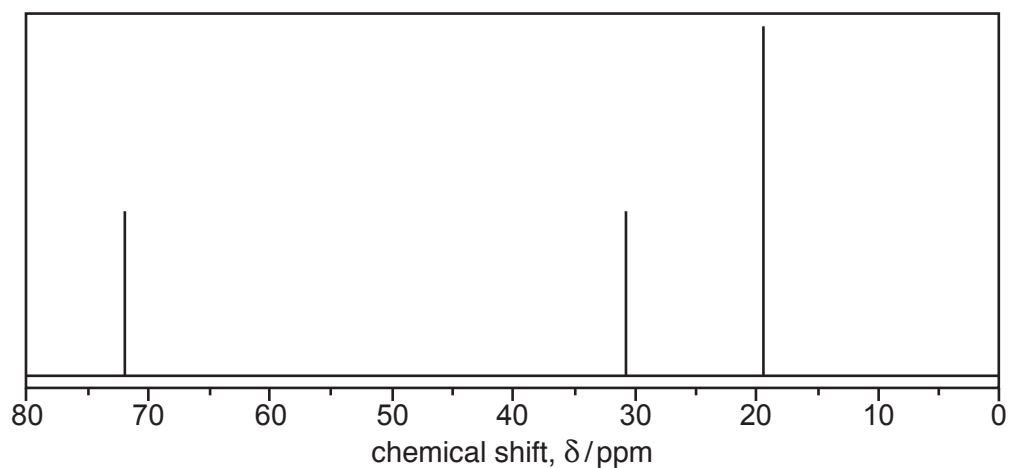
7 Which compound shows 4 peaks in its carbon-13 NMR spectrum?

|          |                                                                                    |
|----------|------------------------------------------------------------------------------------|
| <b>A</b> |   |
| <b>B</b> |   |
| <b>C</b> |   |
| <b>D</b> |  |

Your answer

[1]

- 8 A compound produces the  $^{13}\text{C}$  NMR spectrum below.



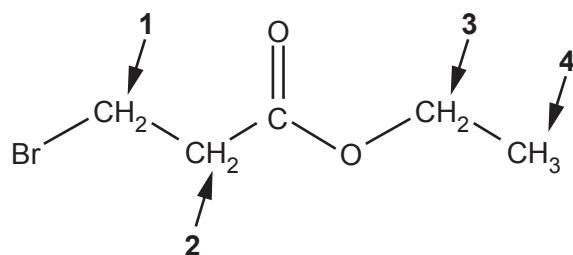
Which compound could have produced this spectrum?

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

Your answer ☐

[1]

- 9 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 |
|--------------------|----------------|-------------------|
| <b>1</b>           |                |                   |
| <b>2</b>           |                |                   |
| <b>3</b>           |                |                   |
| <b>4</b>           |                |                   |

[4]

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

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

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

[1]

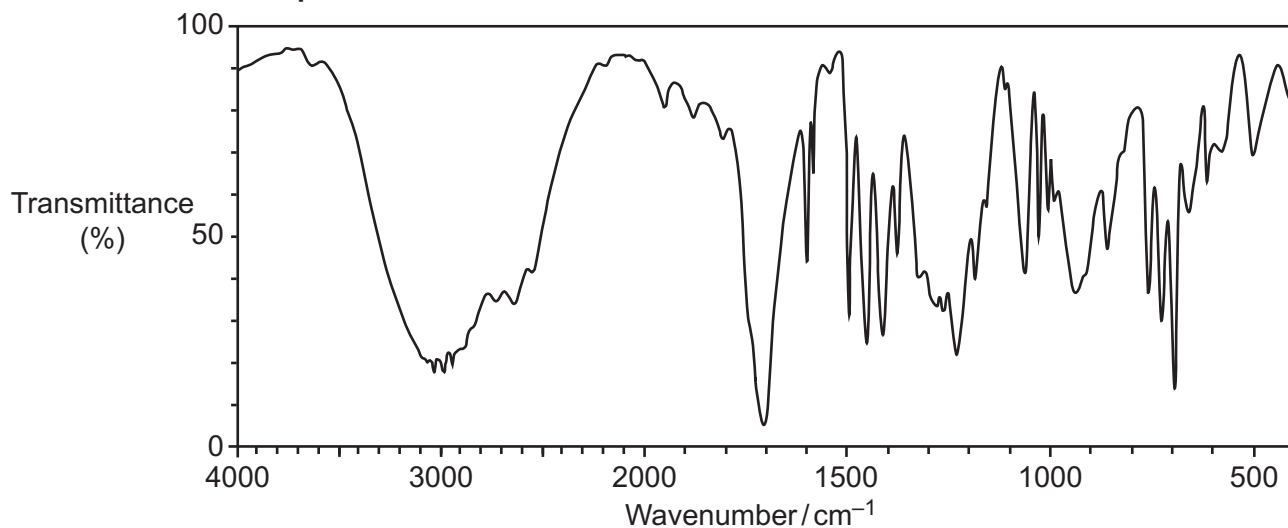
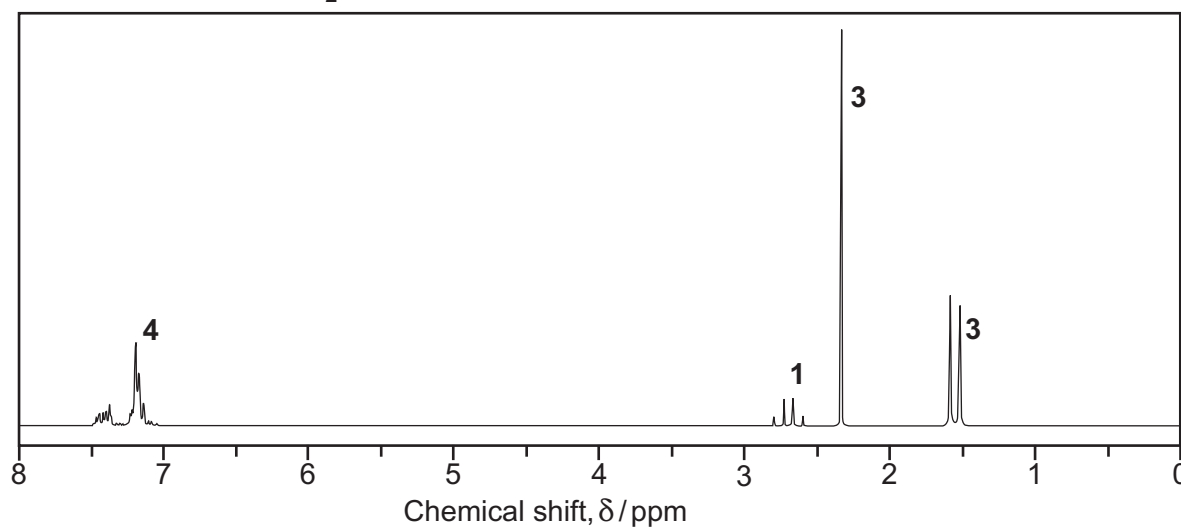
10\* Analysis of an unknown organic compound produced the following results.

**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** **$^1\text{H}$  NMR spectrum in  $\text{D}_2\text{O}$** 

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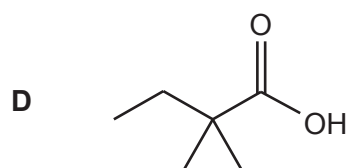
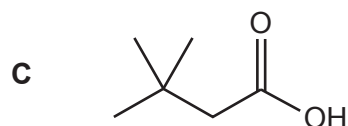
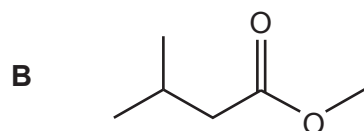
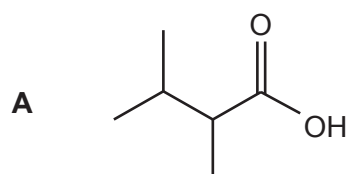
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- 11 Which isomer of  $C_6H_{12}O_2$  produces the smallest number of peaks in its  $^{13}C$  NMR spectrum?

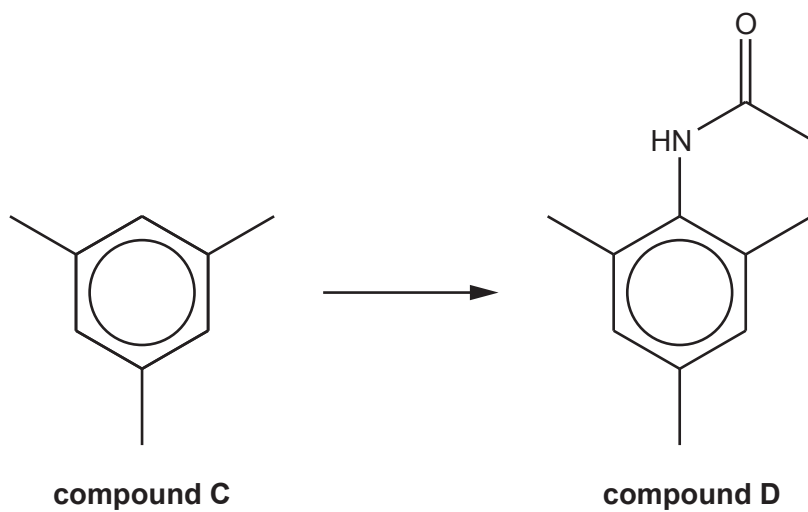


Your answer

[1]

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

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



- 12 Predict the number of peaks in the  $^{13}\text{C}$  NMR spectra of compounds **C** and **D**.

|                        | Compound <b>C</b> | Compound <b>D</b> |
|------------------------|-------------------|-------------------|
| <b>Number of peaks</b> | .....             | .....             |

[2]

- 13 Explain the use of two deuterated compounds in NMR spectroscopy.

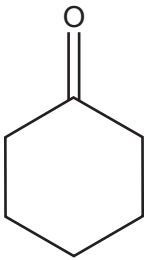
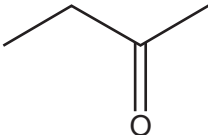
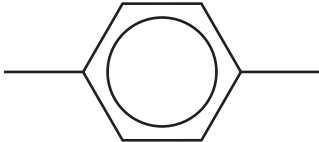
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..... [2]

14 Which compound(s) has/have four peaks in a  $^{13}\text{C}$  NMR spectrum?

|   |                                                                                    |
|---|------------------------------------------------------------------------------------|
| 1 |   |
| 2 |   |
| 3 |  |

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

Your answer

[1]

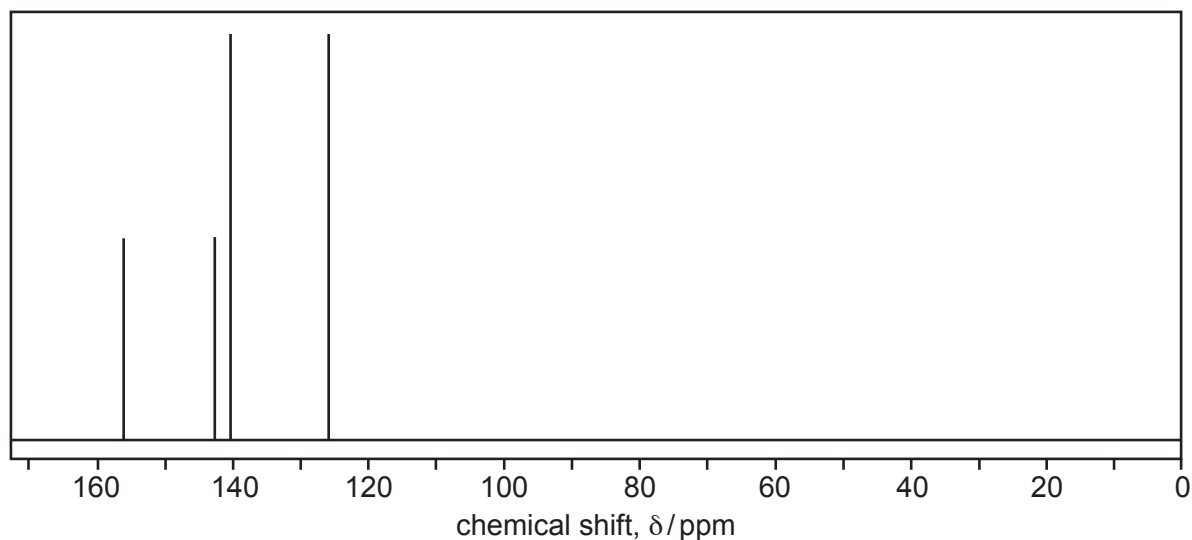
A student reacts phenol with nitric acid and sulfuric acid at 100°C to form impure crystals of an organic compound, **C**. The student purifies the crystals by recrystallisation.

- 15 The pure sample of **C** is analysed to give the following results.

Percentage composition by mass: C, 31.44%; H, 1.31%; N, 18.34%; O, 48.91%.

The mass spectrum of **C** shows a molecular ion peak at  $m/z = 229.0$

The  $^{13}\text{C}$  NMR spectrum of **C** is shown below.



The table shows directing effects for different groups in the electrophilic substitution of aromatic compounds.

| Directing effect | 2- and 4- directing | 3-directing      |
|------------------|---------------------|------------------|
| Group            | –OH                 | –NO <sub>2</sub> |
|                  | –NH <sub>2</sub>    |                  |

Analyse all the information to suggest the structure for **C**.

Show all your reasoning.

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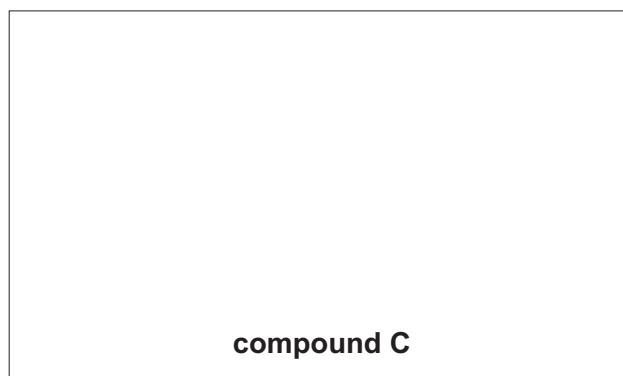
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**[6]**

**Turn over**

- 16\* Compounds **D**, **E** and **F** are isomers with the molecular formula  $C_5H_{10}O$ .  
One of the compounds is alicyclic.

A student carries out test-tube tests on the compounds.  
The observations are shown below.

| Compound | 2,4-DNP            | $H^+/Cr_2O_7^{2-}$ , reflux | Bromine water    |
|----------|--------------------|-----------------------------|------------------|
| <b>D</b> | No change          | Green solution              | No colour change |
| <b>E</b> | Orange precipitate | No colour change            | No colour change |
| <b>F</b> | Orange precipitate | No colour change            | No colour change |

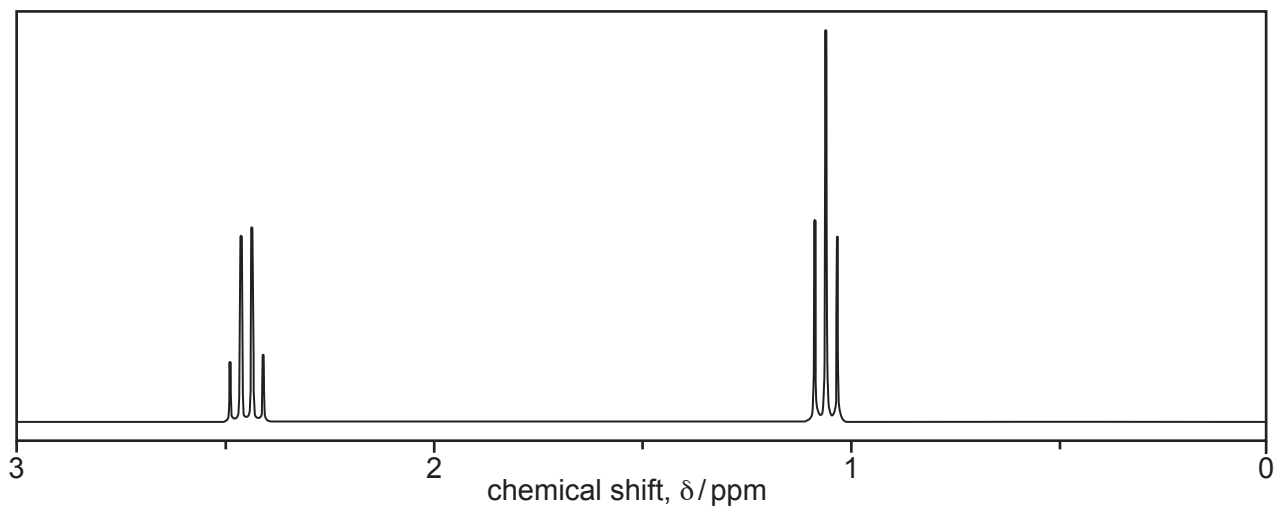
$^{13}C$  NMR spectrum of **D**

Compound **D** has 3 peaks at  $\delta$ /ppm: 24, 36, 73.

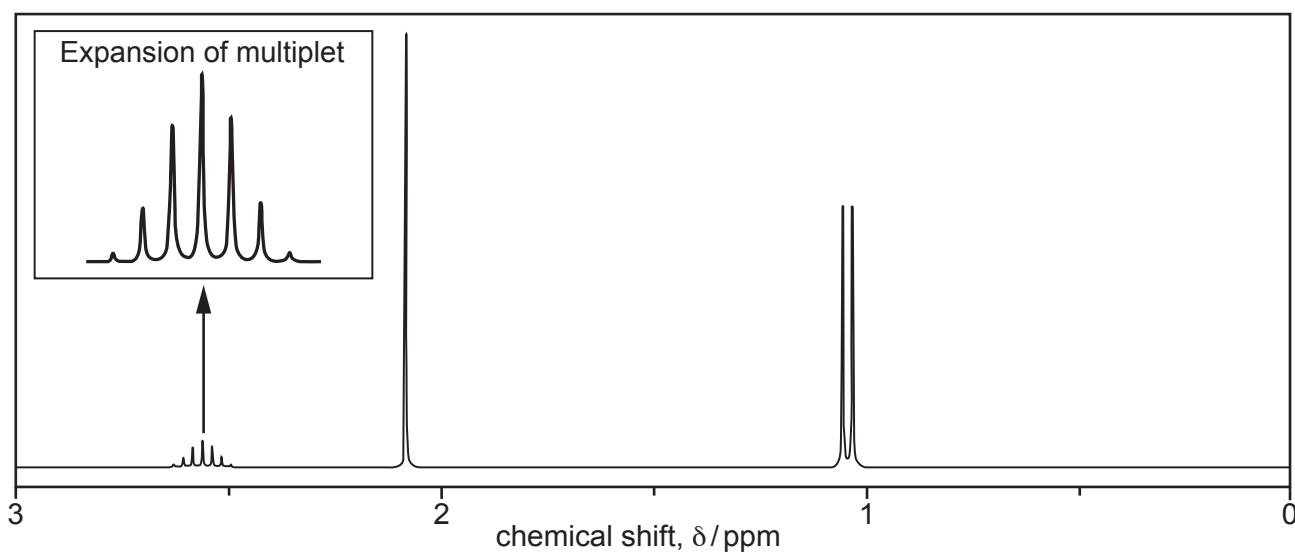
$^1H$  NMR spectra of **E** and **F**

The integration data has been omitted.

Compound **E**



Compound **F**



Analyse the observations and results to identify the structures of **D**, **E** and **F**.

Explain your reasoning.

**[6]**

This image shows a full page of white paper with horizontal blue ruling lines. The lines are evenly spaced and run across the width of the page, providing a template for handwriting practice or general writing. There are no margins, text, or other markings on the page.

Additional answer space if required.

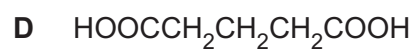
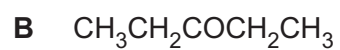
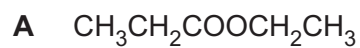
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17 Which compound produces two triplets in its  $^1\text{H}$  NMR spectrum?



Your answer

[1]

18 Which isomer(s) of  $\text{C}_5\text{H}_{12}\text{O}$  has/have 4 peaks in its/their  $^{13}\text{C}$  NMR spectrum?

1 3-methylbutan-2-ol

2 2-methylbutan-2-ol

3 2-methylbutan-1-ol

**A** 1, 2 and 3

**B** Only 1 and 2

**C** Only 2 and 3

**D** Only 1

Your answer

[1]

19 Compounds **D** and **E** are two more structural isomers of  $\text{C}_6\text{H}_{12}$ .

Compounds **D** and **E** do **not** show stereoisomerism.

**Table 16.1** shows NMR and infrared (IR) spectral data for **D** and **E**.

|          | Number of peaks in $^1\text{H}$ NMR spectrum | Number of peaks in $^{13}\text{C}$ NMR spectrum | IR peak at $1620\text{--}1680\text{ cm}^{-1}$ |
|----------|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|
| <b>D</b> | 1                                            | 1                                               | No                                            |
| <b>E</b> | 1                                            | 2                                               | Yes                                           |

**Table 16.1**

Draw the structures of **D** and **E** and explain how the spectral data in **Table 16.1** provides evidence for the structures.

|          |          |
|----------|----------|
|          |          |
| <b>D</b> | <b>E</b> |

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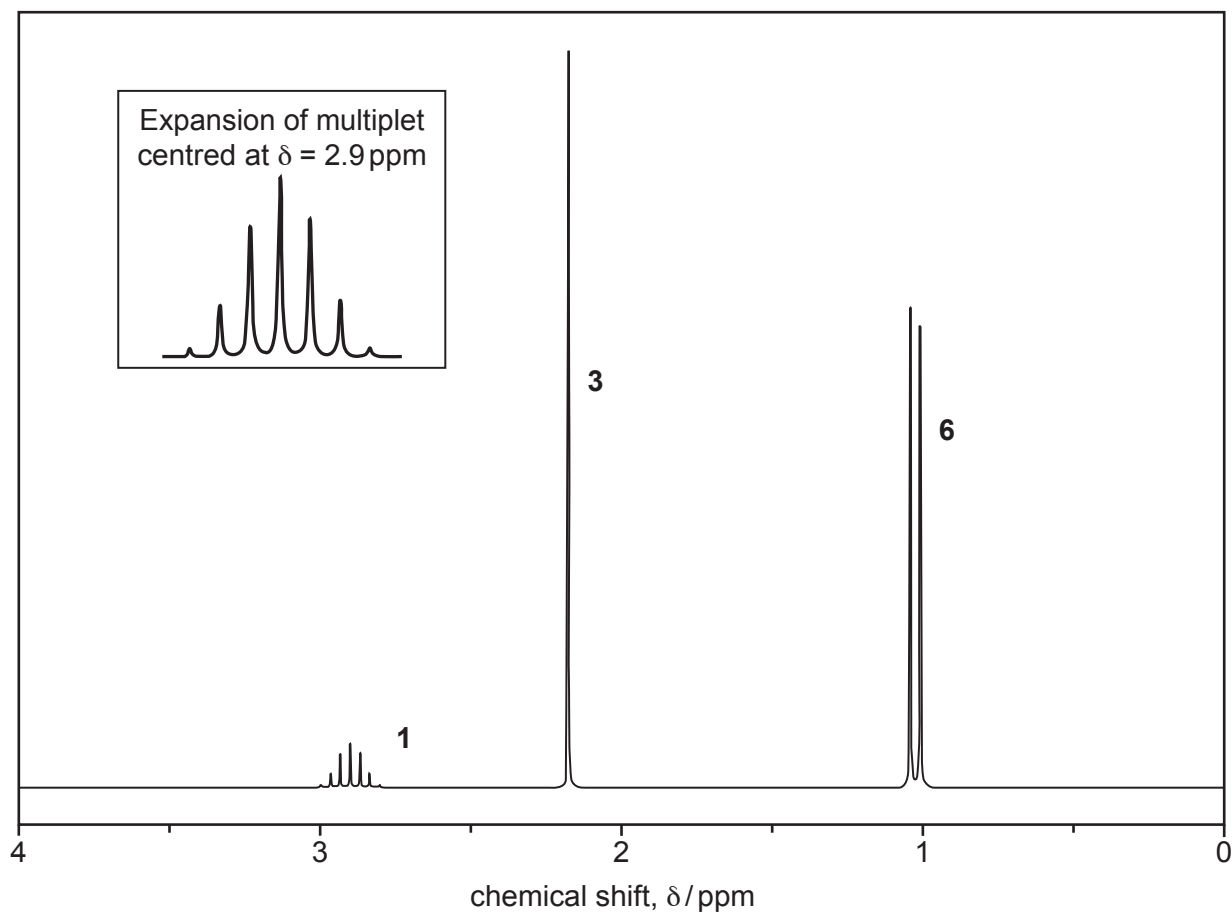
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..... **[4]**

- 20 The organic compound **H** contains carbon, hydrogen and oxygen only and has an  $M_r$  of 114.0.

Compound **H** has two carbonyl groups and no other functional groups.

The  $^1\text{H}$  NMR spectrum of organic compound **H** is shown below.



The numbers by the peaks are the relative peak areas.

Analyse the spectrum to suggest a possible structure for compound **H**.

Show all your reasoning.

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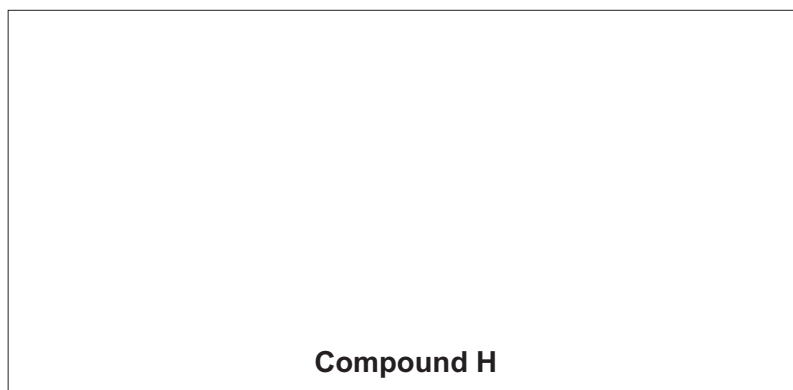
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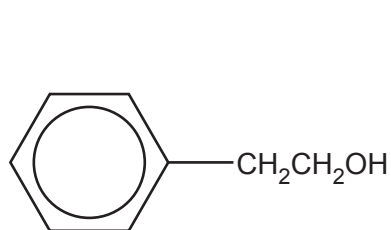
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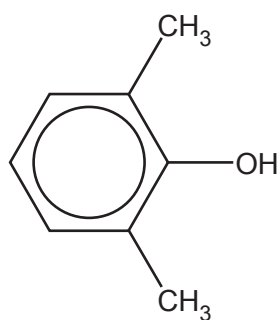
**[4]**

This question is about the chemistry of aromatic compounds.

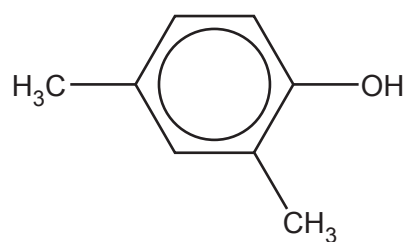
Compounds **J**, **K** and **L**, shown below, are structural isomers.



**Compound J**



**Compound K**



**Compound L**

- 21 A student thought that  $^{13}\text{C}$  NMR spectroscopy could be used to distinguish between compounds **J**, **K** and **L**.

Explain, with reasoning, whether the student is correct.

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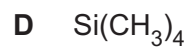
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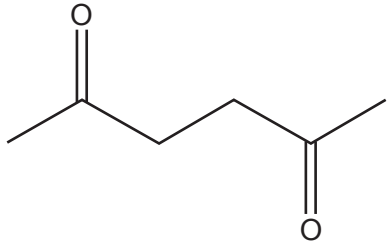
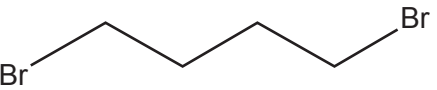
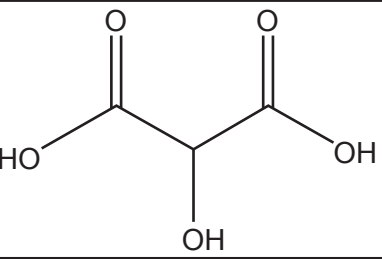
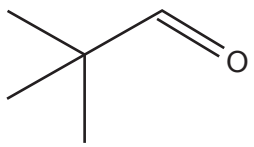
22 Which compound is used for proton exchange in NMR spectroscopy?



Your answer

**[1]**

23 Which compound has the greatest number of peaks in its proton NMR spectrum?

|          |                                                                                    |
|----------|------------------------------------------------------------------------------------|
| <b>A</b> |   |
| <b>B</b> |   |
| <b>C</b> |   |
| <b>D</b> |  |

Your answer

[1]

Source: OCR H432/02 June 2023, original question 17(d)

25\* An unknown organic compound is analysed.

The results are shown below.

**Addition of 2,4-DNP**

No visible change

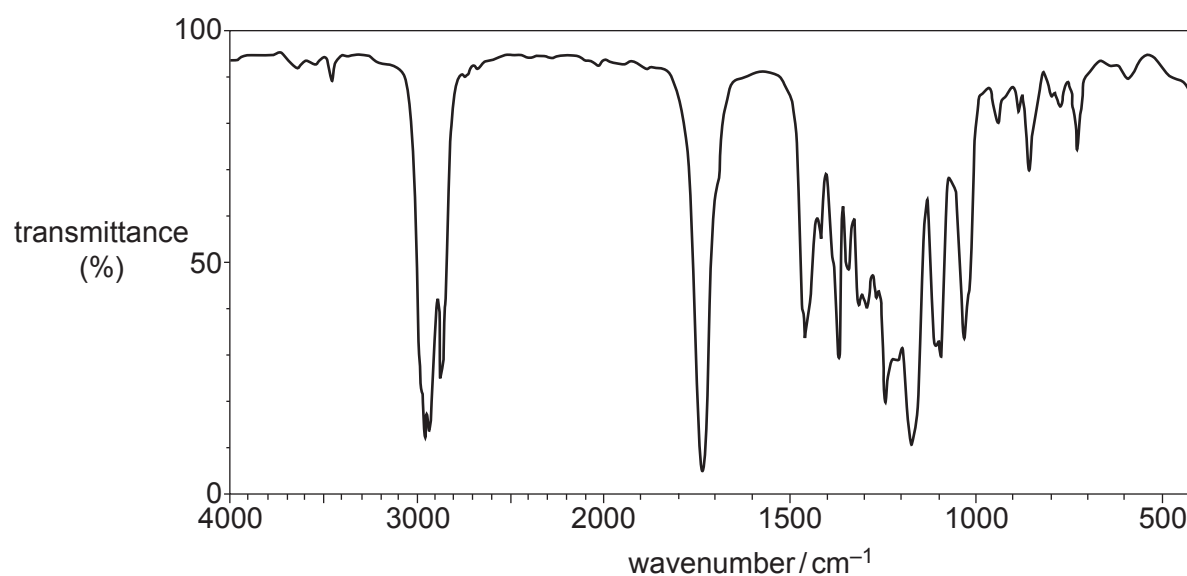
**Elemental analysis by mass**

C, 66.63%; H, 11.18%; O, 22.19%

**Mass spectrum**

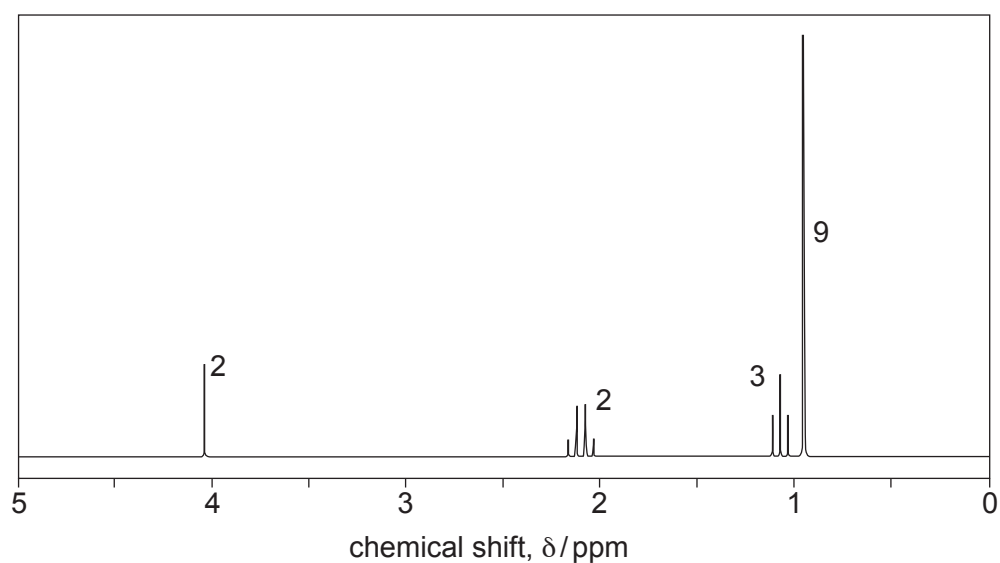
Molecular ion peak at  $m/z = 144.0$

**IR spectrum**



**Proton NMR spectrum**

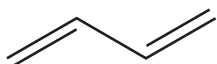
The numbers by each peak are the relative peak areas.



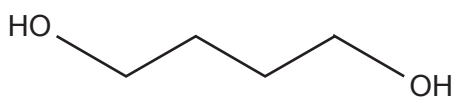


26 The structures of 3 compounds, **1**, **2** and **3**, are shown below.

Which compound(s) would produce a carbon-13 NMR spectrum with 2 peaks?



**1**



**2**



**3**

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

Your answer

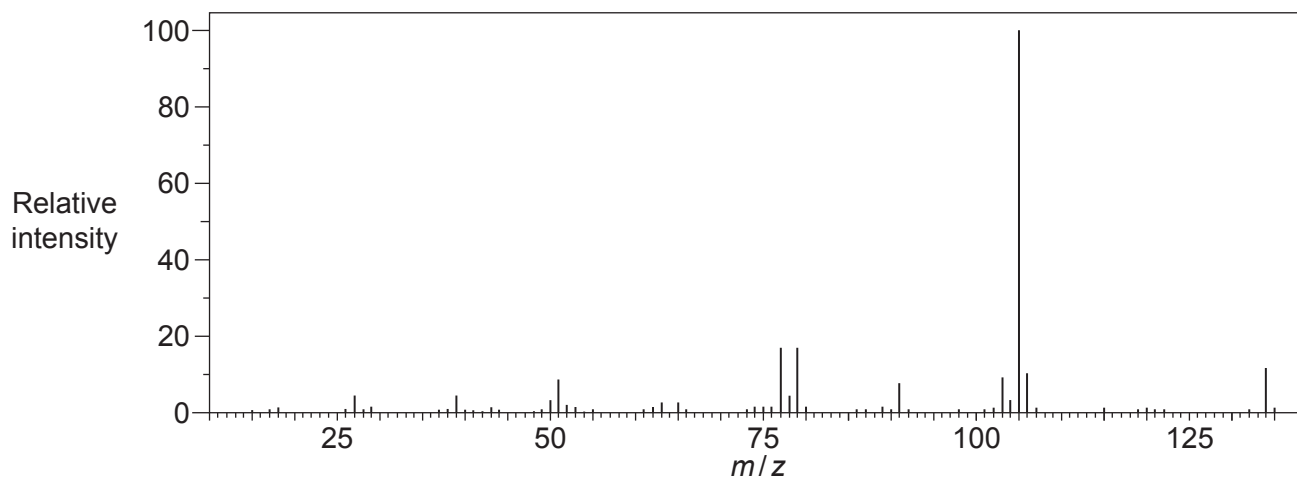
[1]

27\* Analysis of an unknown organic compound **J** produces the following results.

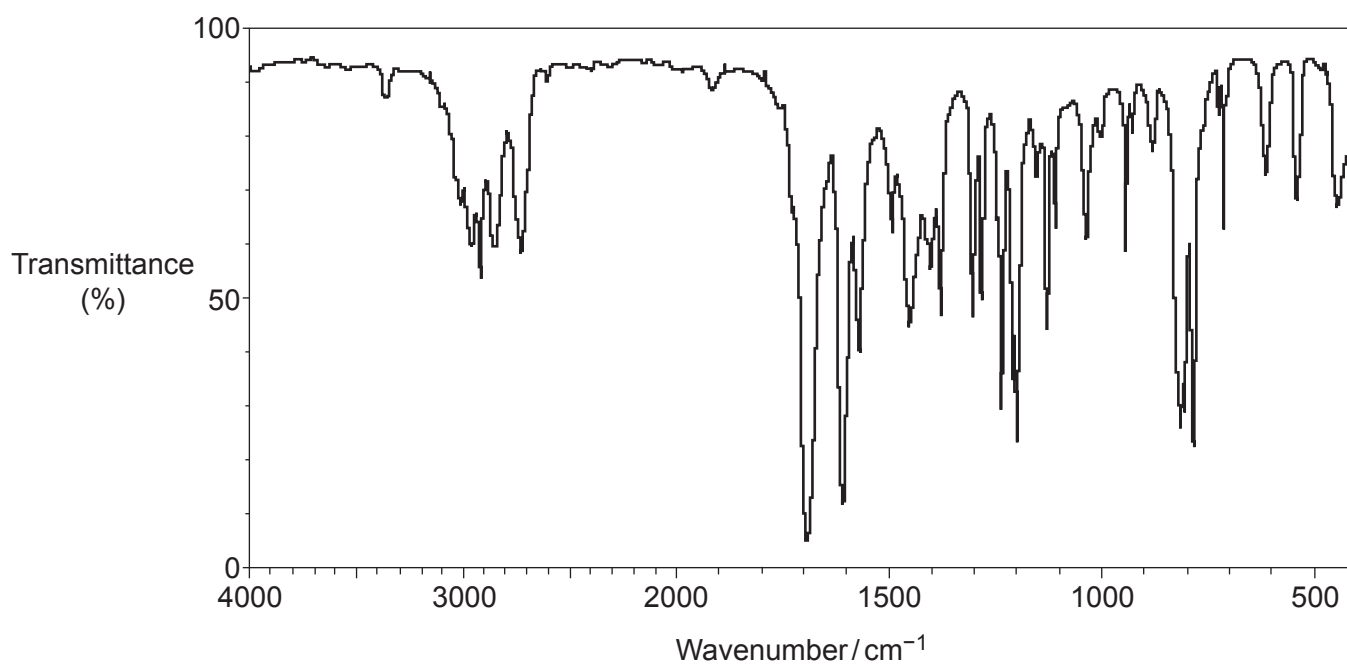
**Elemental analysis by mass of compound J**

C, 80.60%; H, 7.46%; O, 11.94%

**Mass spectrum of compound J**

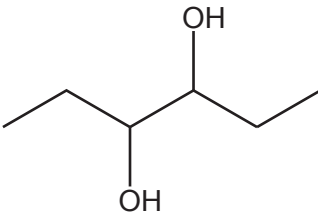
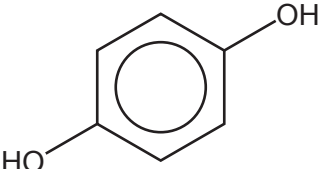
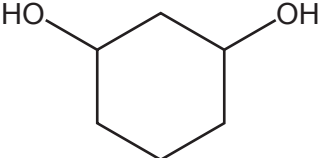


**IR spectrum of compound J**





28 Which compound(s) has/have **three** peaks in their  $^{13}\text{C}$  NMR spectrum?

|   |                                                                                   |
|---|-----------------------------------------------------------------------------------|
| 1 |  |
| 2 |  |
| 3 |  |

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

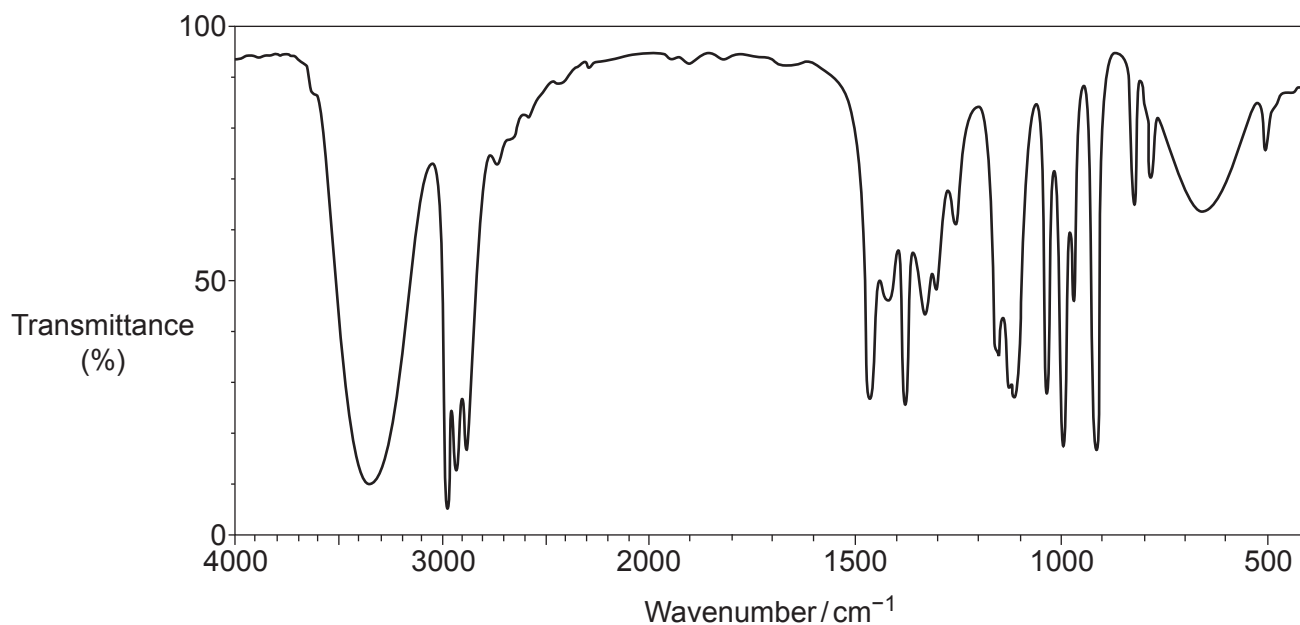
Your answer

[1]

29 This question is about spectral analysis.

- (a) Compound **K**,  $\text{C}_4\text{H}_{10}\text{O}$ , is refluxed with  $\text{H}_2\text{SO}_4$  to form a mixture of compound **L** and compound **M**.

The infrared spectrum of compound **K** is shown.



Compound **L** and compound **M** are analysed using  $^{13}\text{C}$  NMR spectroscopy.

- The  $^{13}\text{C}$  NMR spectrum of compound **L** has 4 peaks.
- The  $^{13}\text{C}$  NMR spectrum of compound **M** has 2 peaks.

Suggest the functional group in compound **K**, showing your reasoning, and suggest possible structures for compound **K**, compound **L** and compound **M**.

Functional group .....

Reasoning .....

|          | Possible structure |
|----------|--------------------|
| <b>K</b> |                    |
| <b>L</b> |                    |
| <b>M</b> |                    |

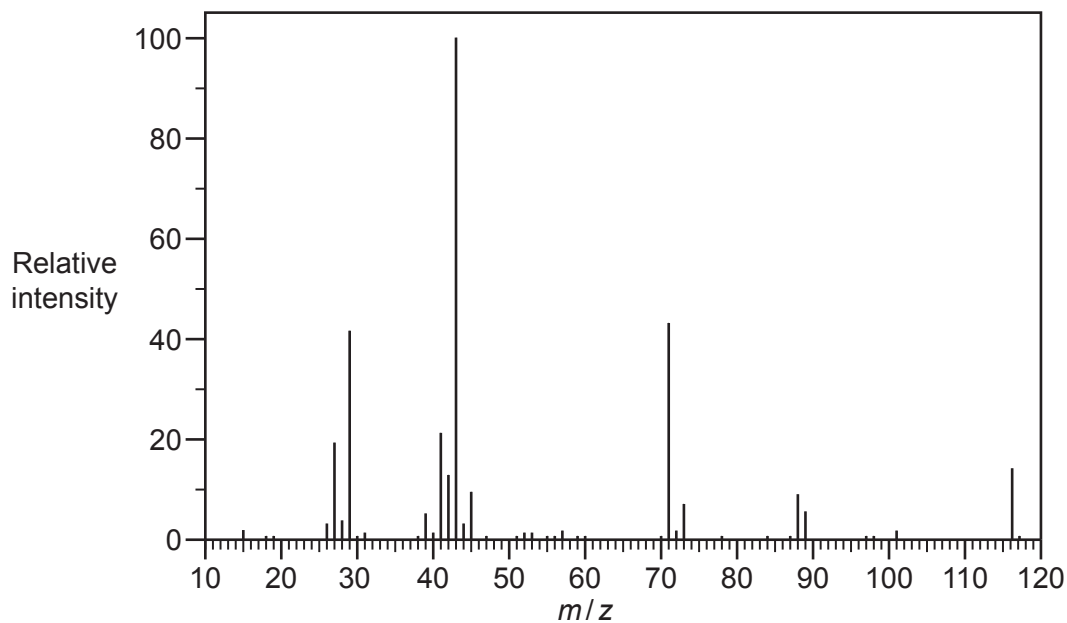
[4]

(b)\* An unknown organic compound **N** is analysed and produces the following results.

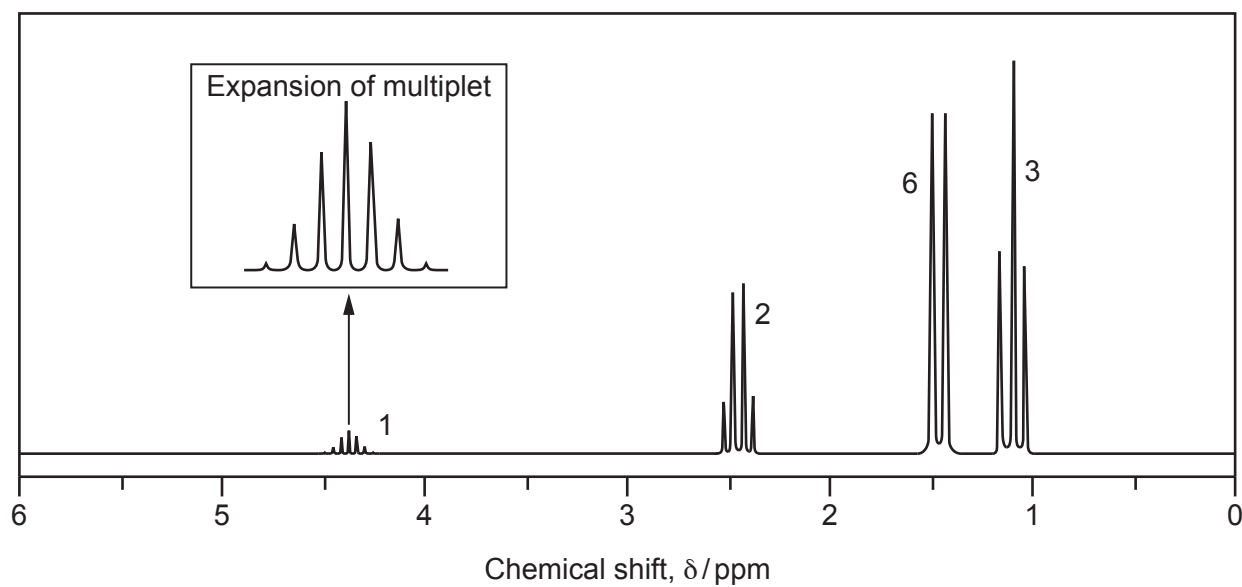
**Elemental analysis by mass**

C, 62.07%; H, 10.34%; O, 27.59%

**Mass spectrum**



**Proton NMR spectrum**



The numbers by the peaks are the relative peak areas.

