Questions

Q1.

This question is about some carbonyl compounds with the molecular formula $C_5H_{10}O$.

An aldehyde with molecular formula $C_5H_{10}O$ has a ^{13}C NMR spectrum with three peaks.

The high resolution ^{1}H NMR spectrum of this aldehyde has two peaks and neither of them is split.

Deduce the **displayed** formula of this aldehyde.
Justify your answer by referring to both NMR spectra.

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(Total for question = 4 marks)

Q2.

Data from the high resolution ^{1}H (proton) NMR spectrum of the ester **Q** are shown in the table.

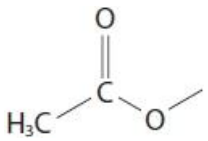
Chemical shift (δ) / ppm	Splitting pattern of peak	Relative peak area
2.50	singlet	3
1.56	quartet	4
1.43	singlet	3
0.92	triplet	6

Part of the structure of **Q** is shown.

Complete the structure of **Q**.

Justify your answer by linking the proton environments in your structure to the relative peak areas and the splitting pattern of the peaks.

(7)



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(Total for question = 7 marks)

Q3.

This question is about the analysis of organic compounds.

There are similarities and differences in the ^{13}C NMR spectra and the high resolution ^{1}H NMR spectra of isomeric
organic compounds.

Compare the NMR spectra of propan-1-ol with those of propan-2-ol.

Include the number of peaks, relative peak areas and splitting patterns, where appropriate.

Chemical shift values are **not** required.

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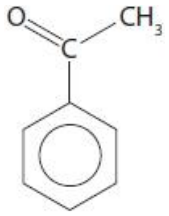
(Total for question = 6 marks)

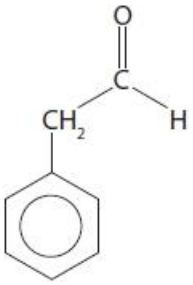
Q4.

Phenylethanone is an ingredient in many types of chewing gum.



One method for the production of phenylethanone involves the reaction of benzene with ethanoyl chloride, CH_3COCl.

Phenylethanone can be distinguished from its structural isomer, phenylethanal, in a number of different ways.



(i) Which would react with phenylethanone but **not** with phenylethanal?

(1)

- ☒ **A** acidified sodium dichromate(VI)
- ☒ **B** alkaline iodine solution
- ☒ **C** Fehling's solution
- ☒ **D** Tollens' reagent

(ii) Give the steps to show how 2,4-dinitrophenylhydrazine could be used to distinguish between phenylethanone and phenylethanal.

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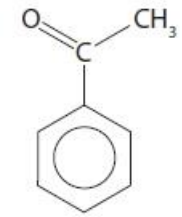
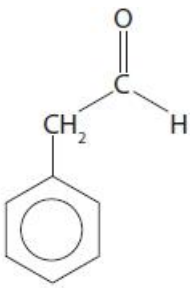
* (iii) Compare and contrast the high resolution proton NMR spectra of phenylethanone and phenylethanal.

You should use the Data Booklet.



Phenylethanone



Phenylethanal

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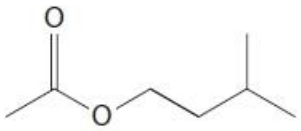
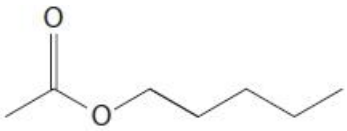
(Total for question = 11 marks)

Q5.

Esters have many uses due to their characteristic aromas and often have common names. For example, isoamyl acetate is referred to as banana oil and amyl acetate has a scent similar to apples.



isoamyl acetate



amyl acetate

What is the number of peaks in a ^{13}C NMR spectrum of isoamyl acetate and of amyl acetate?

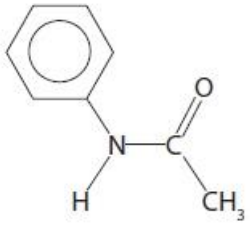
(1)

		isoamyl acetate	amyl acetate
☒	**A**	5	6
☒	**B**	6	6
☒	**C**	6	7
☒	**D**	7	7

(Total for question = 1 mark)

Q6.

Antifebrin was the trade name for N-phenylethanamide which was used as a painkiller until paracetamol was discovered.



Antifebrin

What is the number of peaks in a C-13 NMR spectrum of Antifebrin?

(1)

- ☒ **A** 5
- ☒ **B** 6
- ☒ **C** 7
- ☒ **D** 8

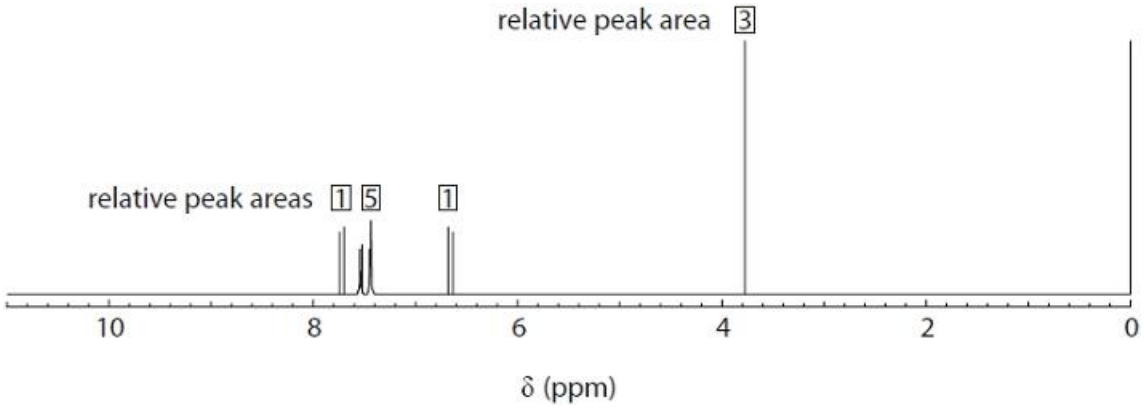
(Total for question = 1 mark)

Q7.

Methyl cinnamate, $C_{10}H_{10}O_2$, is a white crystalline solid used in the perfume industry.

A sample of methyl cinnamate was analysed by high resolution proton NMR spectroscopy.

A simplified spectrum is shown.



(i) Name the compound responsible for the peak at a chemical shift of 0 ppm, stating its purpose.

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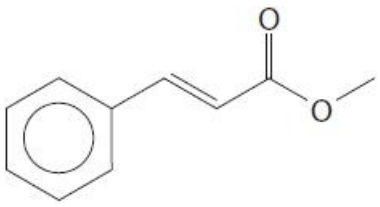
(ii) Identify the proton environment that causes the peak at a chemical shift of 3.8 ppm by circling it on

the diagram shown. Fully justify your answer.

(3)



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(Total for question = 5 marks)

Q8.

This question is about the use of NMR spectroscopy to distinguish between isomers of $C_6H_{12}O_2$.

(i) There are three other isomers of $C_6H_{12}O_2$ which are carboxylic acids with **five** peaks in their **carbon-13** NMR spectra.

Draw the structural formula of **two** of these isomers.

(2)

(ii) Draw the **skeletal** formula of a cyclic diol isomer of $C_6H_{12}O_2$ that has only **two** peaks in its **carbon-13** NMR spectrum.

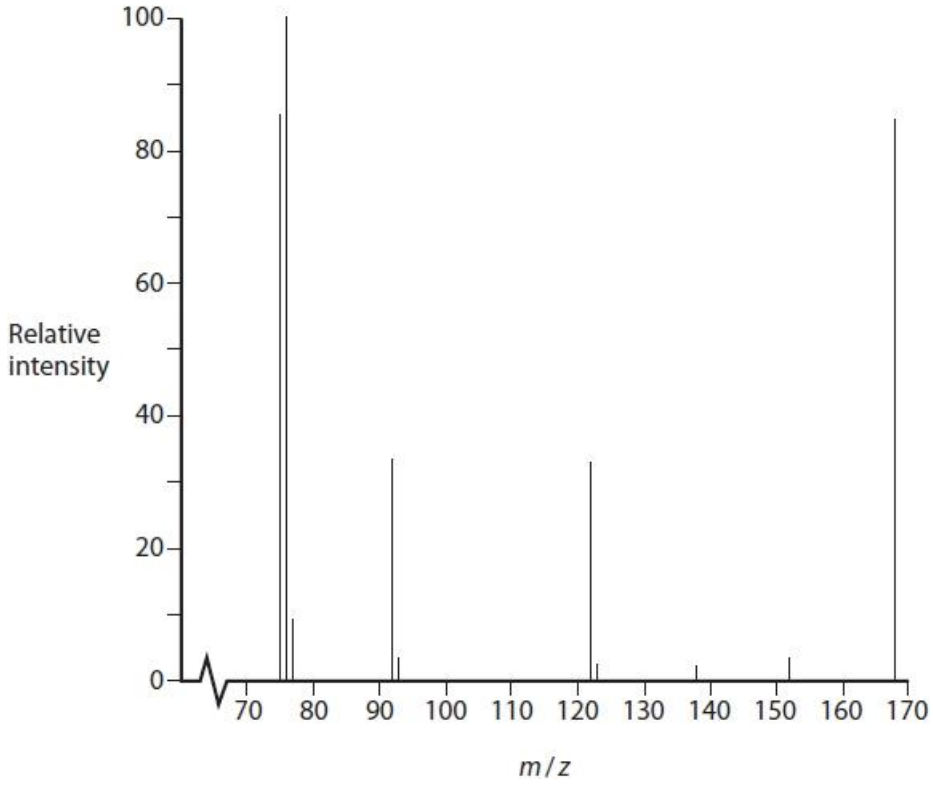
(1)

(Total for question = 3 marks)

Q9.

Organic compound **D** contains the elements carbon, hydrogen, oxygen and nitrogen only.

Part of the mass spectrum of **D** is shown.



Compound **D** contains a benzene ring.

(i) Give the molecular formula of the species that causes the peak at *m* / *z* = *76* in the mass spectrum of **D**.

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(1)

(ii) Draw the structures of the **three** possible isomers of **D** containing a benzene ring.

(2)

(iii) The ^{13}C NMR spectrum of compound **D** has four peaks.

Identify the structure of **D**. Justify your answer by labelling the different carbon environments in **all** the structures drawn in (ii).

(3)

(Total for question = 6 marks)

Q10.

This question is about the use of NMR spectroscopy to distinguish between isomers of $C_6H_{12}O_2$.

Tetramethylsilane (TMS) is a compound used as a standard when recording both ^{1}H and ^{13}C NMR spectra.

(i) Give the structural formula of TMS.

(1)

(ii) TMS is an inert and non-toxic compound. State **two** other reasons why TMS is suitable for use as a standard when recording NMR spectra.

(2)

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(Total for question = 3 marks)

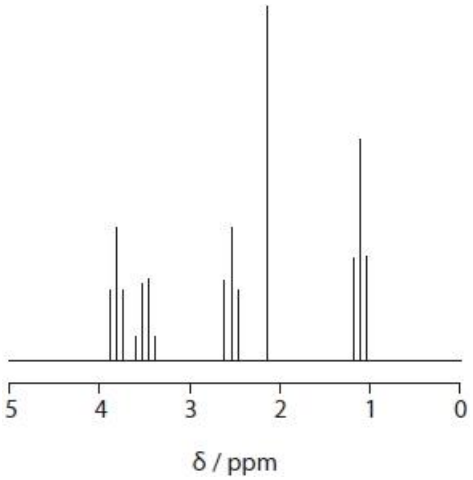
Q11.

This question is about the use of NMR spectroscopy to distinguish between isomers of $C_6H_{12}O_2$.

(i) Draw the structural formulae of the **two** esters with formula $C_6H_{12}O_2$ that each have only **two** peaks, both singlets, in their high resolution **proton** NMR spectra. The relative peak areas are 3:1 for both esters.

(2)

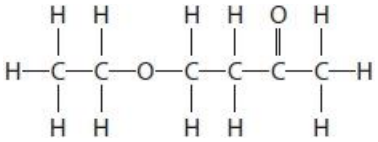
(ii) The high resolution **proton** NMR spectrum of another isomer of $C_6H_{12}O_2$ is shown.



The ratios of the number of protons for the five sets peaks in the spectrum are given in the table.

δ / ppm	3.8	3.5	2.6	2.2	1.2
Ratio of the number of protons	2	2	2	3	3

Show that **all** these data are consistent with the displayed formula shown. Refer to the five chemical shifts and explain **two** of the splitting patterns.



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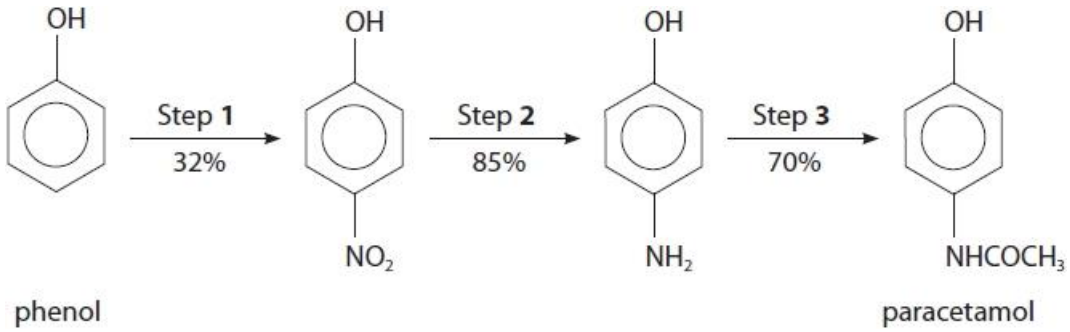
(Total for question = 7 marks)

Q12.

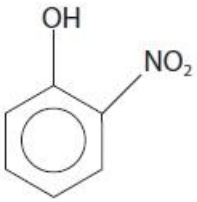
The painkiller paracetamol can be synthesised from phenol in three steps.
The percentage yield for each step is shown.



In Step **1** another product also forms. The two products can be distinguished using their ^{13}C NMR spectra.

Complete the table to show the number of peaks in each ^{13}C NMR spectrum.

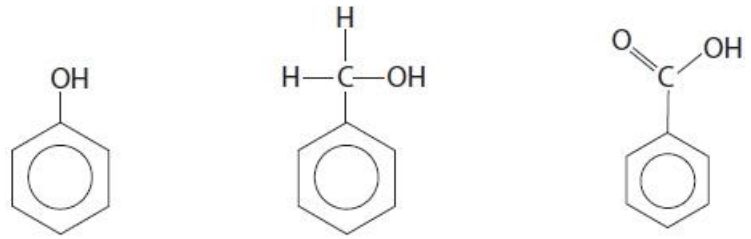
(2)

Product		
Number of peaks in the ^{13}C NMR spectrum		

(Total for question = 2 marks)

Q13.

This is a question about the analysis of three aromatic substances with —OH groups.



phenol phenylmethanol benzoic acid

Spectroscopy is an effective means of distinguishing between molecules.

(i) Compare and contrast the infrared spectra of phenol, phenylmethanol and benzoic acid. Include relevant bonds and their wavenumber ranges using the Data Booklet.

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(ii) Predict the number of peaks present, and their chemical shifts, in the ^{13}C nuclear magnetic resonance (NMR) spectrum of
phenylmethanol.
Use the information in the Data Booklet to help you.

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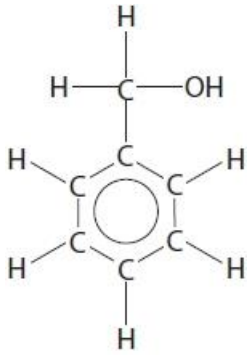

phenylmethanol

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(iii) Give the formula of a fragment ion, with its *m*/*z* value, that you would expect to be present in the mass spectrum of
benzoic acid but **not** in the mass spectrum of phenol or the mass spectrum of phenylmethanol.

(2)

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(Total for question = 10 marks)