



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 1H 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)



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 ^1H 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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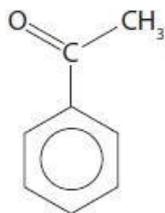
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(Total for question = 6 marks)



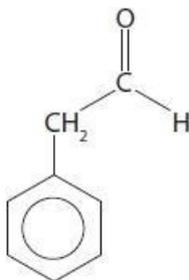
Q4.

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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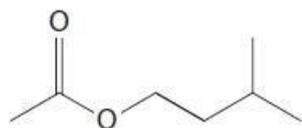
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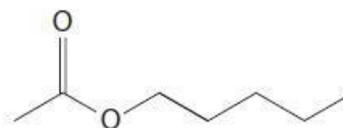


Q5.

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)

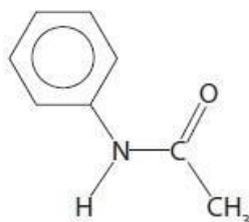
	isoamyl acetate	amyl acetate
<input type="checkbox"/> A	5	6
<input type="checkbox"/> B	6	6
<input type="checkbox"/> C	6	7
<input type="checkbox"/> D	7	7

(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)

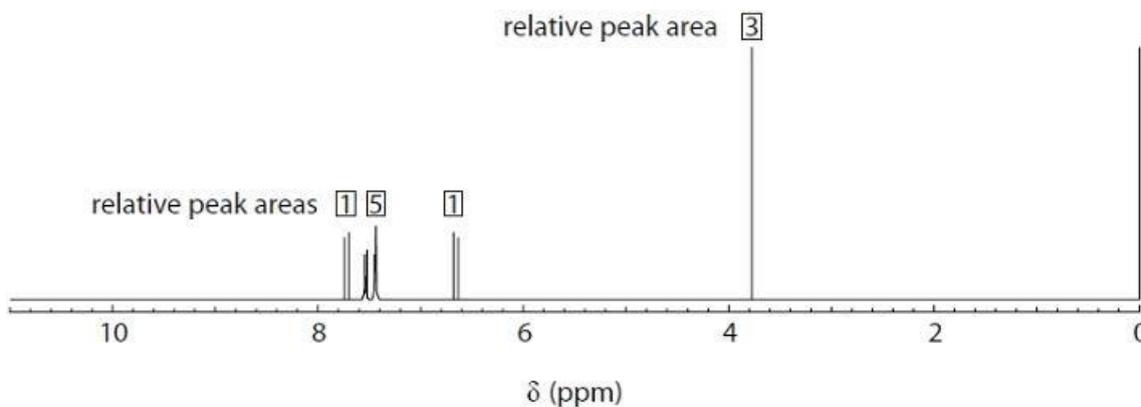


Q7.

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.

(2)

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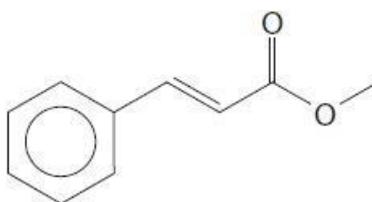
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(ii) Identify the proton environment that causes the peak at a chemical shift of 3.8 ppm by circling it on

the diagram shown. Fully justify your answer.

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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)

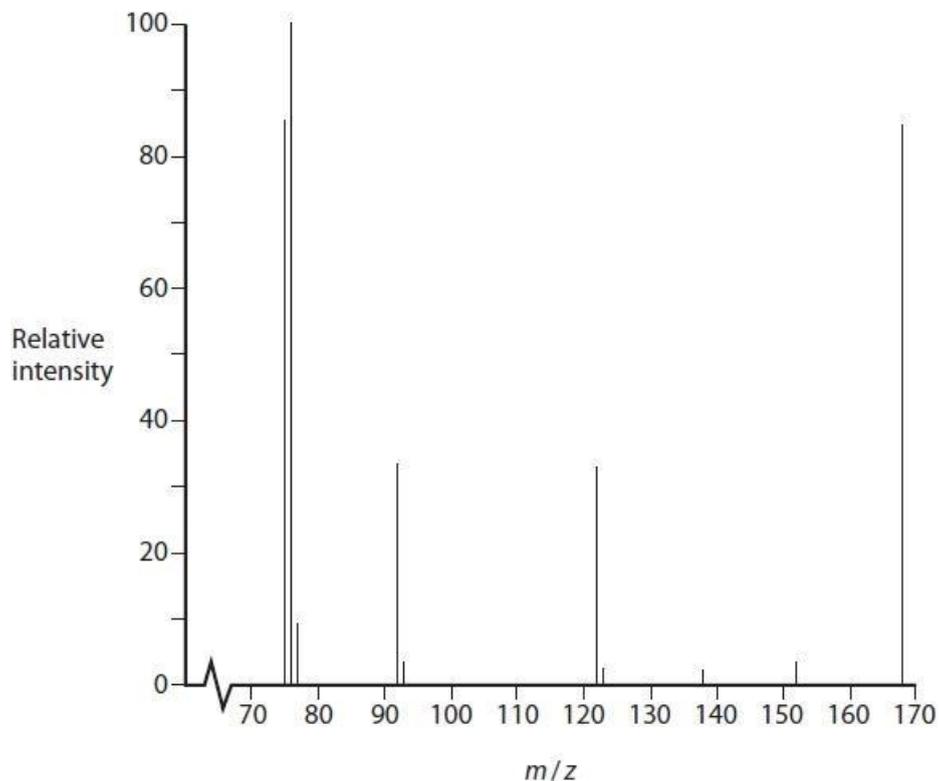
(Total for question = 3 marks)



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 1H 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.

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(Total for question = 3 marks)



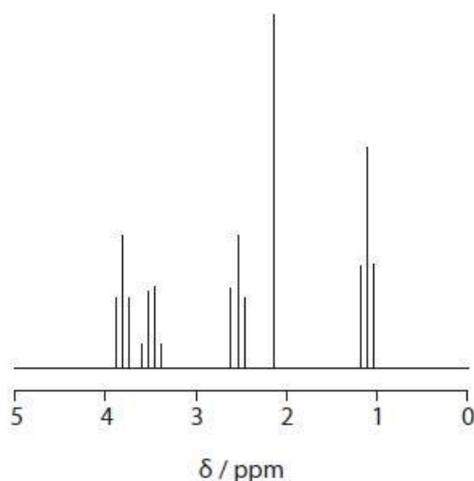
Q11.

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.

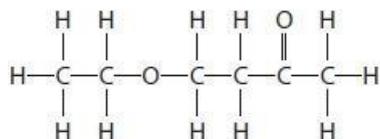


The ratios of the number of protons for the five sets peaks in the spectrum are given in the table.

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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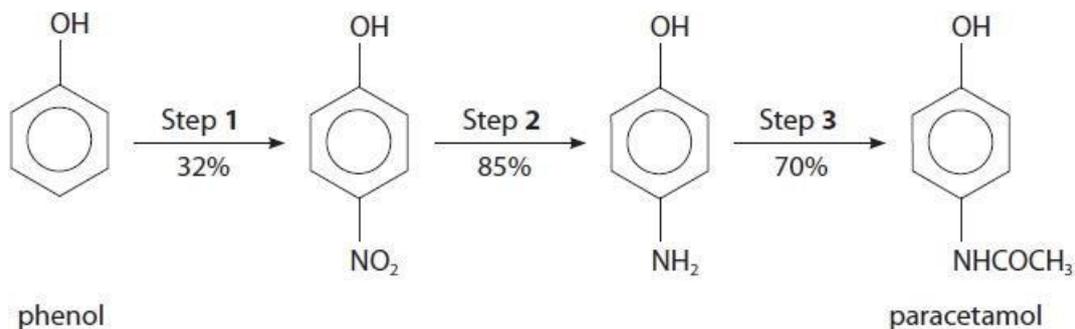
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(Total for question = 7 marks)



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		

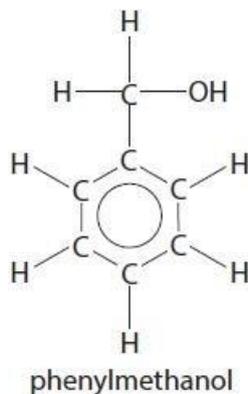
(Total for question = 2 marks)



(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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(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.

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(Total for question = 10 marks)