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.

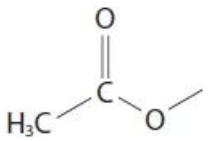
Chemical shift (δ) / ppm	Splitting pattern of peak	Relative peak area
2.50	singlet	3
1.56	quartet	4
1.43	singlet	3
0.92	triplet	6

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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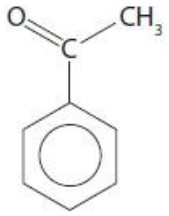
(Total for question = 6 marks)

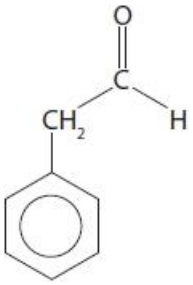
Q4.

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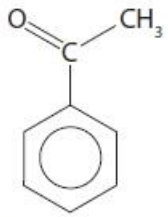
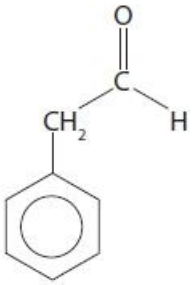
* (iii) Compare and contrast the high resolution proton NMR spectra of phenylethanone and phenylethanal.

You should use the Data Booklet.



Phenylethanone



Phenylethanal

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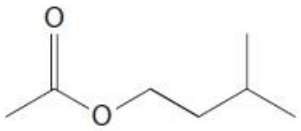
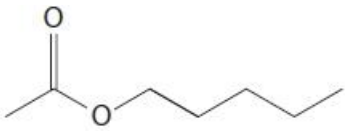
(Total for question = 11 marks)

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?

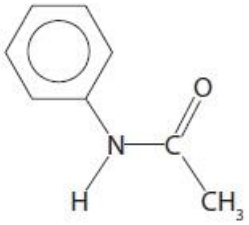
(1)

		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

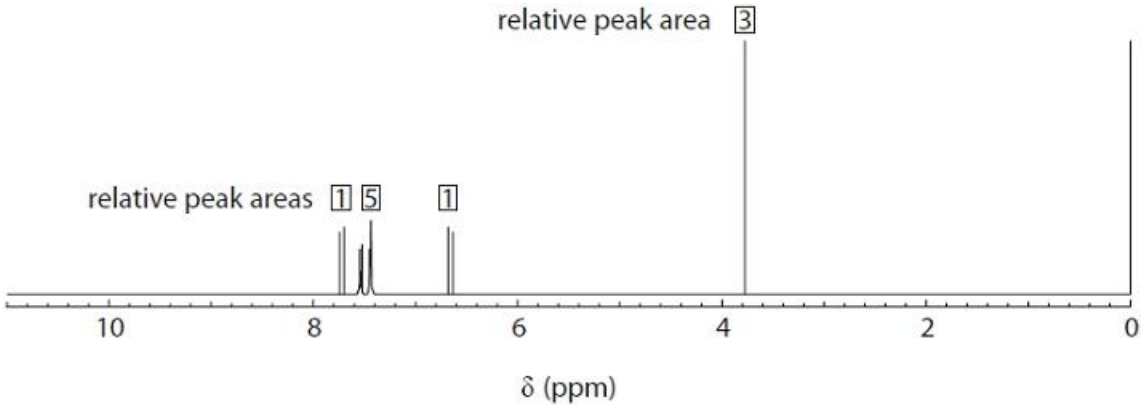
(Total for question = 1 mark)

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.

(2)

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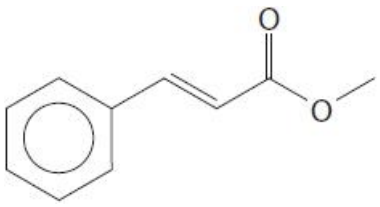
(ii) Identify the proton environment that causes the peak at a chemical shift of 3.8 ppm by circling it on

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.

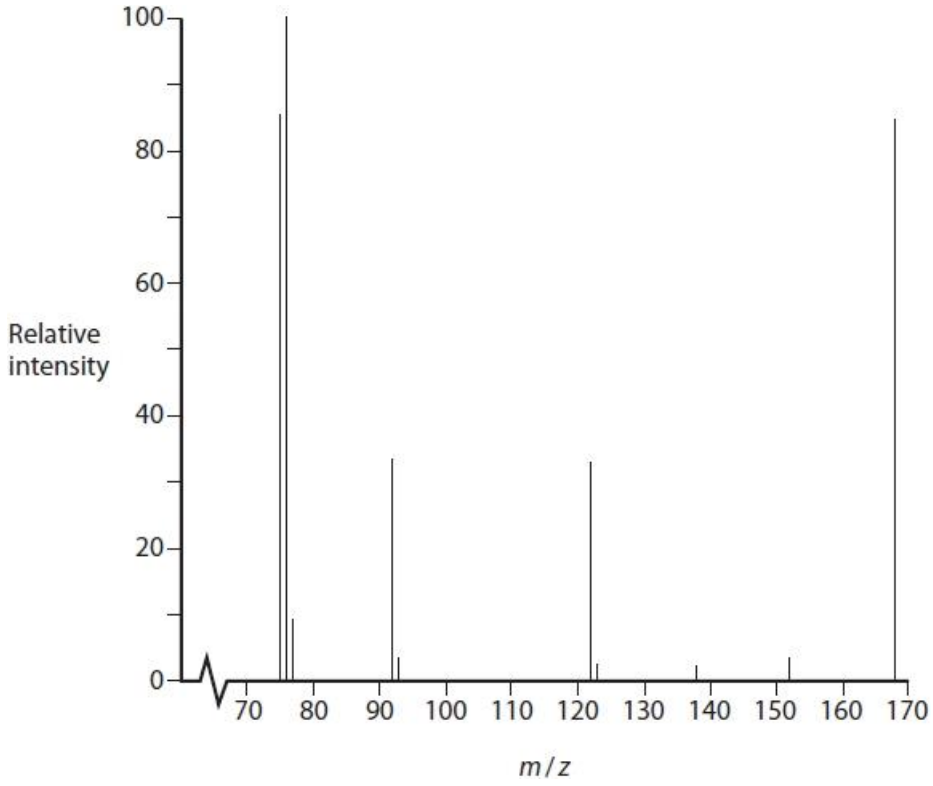
(1)

(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)

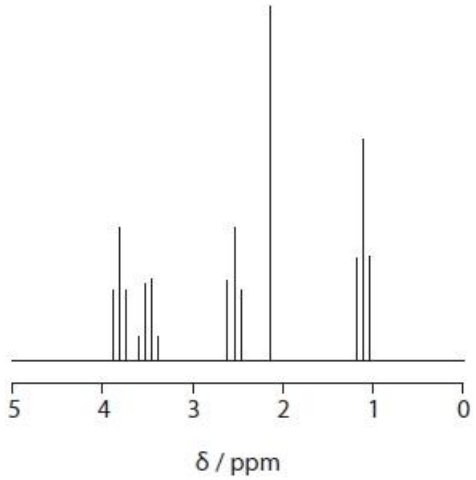
Q11.

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)

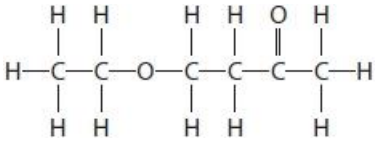
(ii) The high resolution **proton** NMR spectrum of another isomer of $C_6H_{12}O_2$ is shown.



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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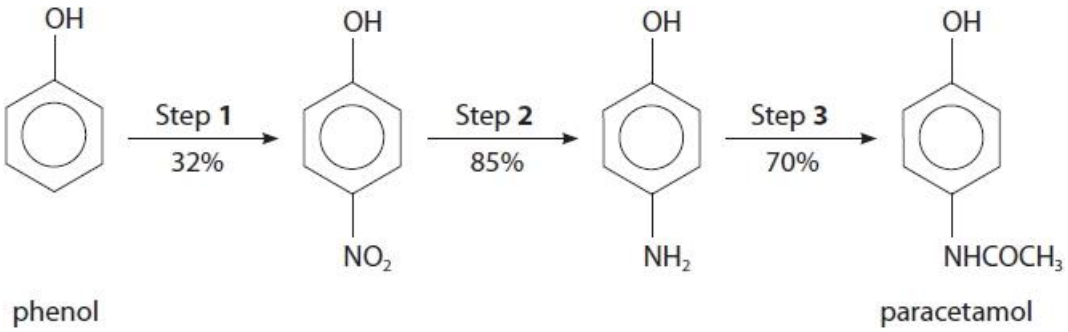
(Total for question = 7 marks)

Q12.

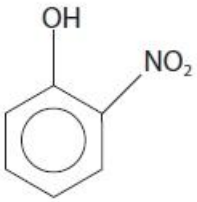
The painkiller paracetamol can be synthesised from phenol in three steps.
The percentage yield for each step is shown.



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.

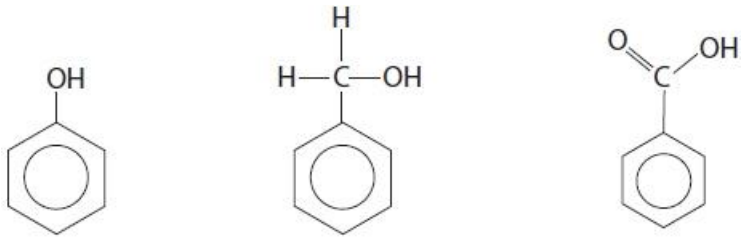
(2)

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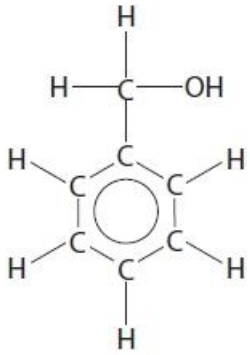
(ii) Predict the number of peaks present, and their chemical shifts, in the ^{13}C nuclear magnetic resonance (NMR) spectrum of
phenylmethanol.
Use the information in the Data Booklet to help you.

(3)



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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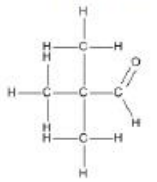
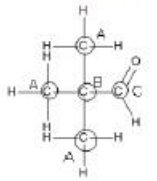
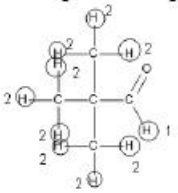
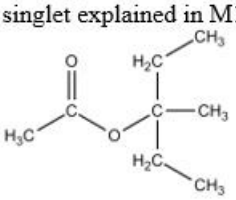
(Total for question = 10 marks)

Mark Scheme

Q1.

Question Number	Answer	Additional Guidance	Mark
	An answer that makes reference to the following points: • displayed formula of aldehyde (1) • three different carbon environments indicated (1) • two different proton environments indicated (1) • no splitting as there are no hydrogens on the adjacent carbon atom(s)	Example of displayed formula:  Allow CH_3 groups but aldehyde group must be displayed Example of three carbon environments:  Example of two proton environments:  Stand alone mark	(4)

Q2.

Question Number	Answer	Additional Guidance	Mark
	An answer that makes reference to the following points: **Peak at 2.50 ppm** • identified as C**H**$_3$CO (as relative peak area = 3 / singlet so no protons on adjacent C) **(1)** **Peak at 1.56 ppm** • 2 C**H**$_2$ groups as relative peak area = 4 **(1)** • (the 2 C**H**$_2$ groups / hydrogen environment) next to CH_3 groups as peak is a quartet **(1)** **Peak at 0.92 ppm** • 2 C**H**$_3$ groups as relative peak area = 6 **(1)** • (the 2 C**H**$_3$ groups / hydrogen environment) next to CH_2 groups as peak is a triplet **(1)** **Peak at 1.43 ppm** • C**H**$_3$ group with no protons on adjacent carbon atoms as (relative peak area = 3 and) singlet **(1)** • structure of **Q** **(1)**	Allow credit for annotations on table in p14 and on labelled structures Allow adjacent protons / hydrogens for protons on adjacent C Penalise H^+ for protons once only Allow ester group / H-C-C=O / CH_3 on left of structure given is indicated Do not award if aldehyde / ketone mentioned Allow 4 protons / hydrogens Allow 6 protons / hydrogens Allow just CH_3 identified in M6 if singlet explained in M1 	(7)

Q3.

Acceptable Answers	Additional Guidance	Mark
This question assesses a student's ability to show a coherent and logically structured answer with linkages and fully-sustained reasoning. Marks are awarded for indicative content and for how the answer is structured and shows lines of reasoning. The following table shows how the marks should be awarded for indicative content. Number of indicative marking points seen in answer / Number of marks awarded for indicative marking points 6 / 4 5-4 / 3 3-2 / 2 1 / 1 0 / 0 Guidance on how the mark scheme should be applied: The mark for indicative content should be added to the mark for lines of reasoning. For example, an answer with five indicative marking points that is partially structured with some linkages and lines of reasoning scores 4 marks (3 marks for indicative content and 1 mark for partial structure and some linkages and lines of reasoning). If there are no linkages between points, the same five indicative marking points would yield an overall score of 3 marks (3 marks for indicative content and no marks for linkages). The following table shows how the marks should be awarded for structure and lines of reasoning.		(6)

		Number of marks awarded for structure of answer and sustained line of reasoning		
	Answer shows a coherent and logical structure with linkages and fully sustained lines of reasoning demonstrated throughout.	2		
	Answer is partially structured with some linkages and lines of reasoning.	1		
	Answer has no linkages between points and is unstructured.	0		
	Comment: Look for the indicative marking points first, then consider the mark for structure of answer and sustained line of reasoning		In general it would be expected that 5 or 6 indicative points would get 2 reasoning marks, and 3 or 4 indicative points would get 1 mark for reasoning, and 0, 1 or 2 indicative points would score zero marks for reasoning.	

	Indicative content • **IP1 -** Similarity **both** ^{1}H NMR spectra have a peak (which is a singlet with relative peak area 1) for OH • **IP2 -** ^{13}C spectra 3 peaks for propan-1-ol **and** 2 peaks for propan-2-ol	**General points to note** If there is any incorrect chemistry, deduct mark(s) from the reasoning. If no reasoning mark(s) awarded do not deduct mark(s). e.g. Mention of splitting on the ^{13}C spectra Deduct 1 reasoning mark if the similarity in IP1 has not been explicitly mentioned All IP can be shown on clearly labelled diagrams of structures and/or spectra Allow carbon environments for peaks Ignore any reference to peak areas	

	• **IP3 -** ^{1}H spectra number of peaks 4 peaks for propan-1-ol **and** 3 peaks for propan-2-ol		
	• **IP4 -** ^{1}H spectra relative peak areas (relative) peak areas 3 : 2 : 2 : 1 for propan-1-ol, 6 : 1 : 1 for propan-2-ol	Allow ratios in any order e.g. 1 : 2 : 2 :3	
	• **IP5 -** ^{1}H splitting pattern for propan-1-ol 2 triplets, 1 sextet / split into 6 and 1 singlet	Allow hextet for sextet Ignore missing singlet if this has been given in similarity	
	• **IP6 -** ^{1}H splitting pattern for propan-2-ol 1 doublet, 1 septet / split into 7 and 1 singlet	Allow heptet for septet Ignore missing singlet if this has been given in similarity	

Q4.

Question Number	Answer	Mark
(i)	**The only correct answer is B** (alkaline iodine solution) ***A*** *is not correct because this oxidising agent would react with phenylethanal and not with phenylethanone which is the wrong way round* ***C*** *is not correct because test is for aldehydes and so would react with phenylethanal and not with phenylethanone which is the wrong way round* ***D*** *is not correct because test is for aldehydes and so would react with phenylethanal and not with phenylethanone which is the wrong way round*	**(1)**

Question Number	Answer	Additional Guidance	Mark
(ii)	An answer that makes reference to the following points: • formation of yellow/orange/red (crystalline) precipitate **(1)** • (Filter then) recrystallisation of products **(1)** • determination of melting temperature **(1)** • comparison (and hence identification) from use of database/known values **(1)**	Colour and state are both required Allow solid for ppt Ignore any conditions given with the use of 2,4-DNPH Penalise M3 if any reference to boiling temperature Award only in the context of melting temperature of the hydrazones or as a TE of boiling temperature Max 3 out of 4 if test is only carried out with one of the carbonyls	**(4)**

<table>
<tr><th>Question Number</th><th>Answer</th><th>Additional Guidance</th><th>Mark</th></tr>
<tr>
<td>* (iii)</td>
<td>
This question assesses the student's ability to show a coherent and logically structured answer with linkages and fully sustained reasoning.

Marks are awarded for indicative content and for how the answer is structured and shows lines of reasoning.

The following table shows how the marks should be awarded for indicative content.
<table>
<tr><th>Number of indicative marking points seen in answer</th><th>Number of marks awarded for indicative marking points</th></tr>
<tr><td>6</td><td>4</td></tr>
<tr><td>5-4</td><td>3</td></tr>
<tr><td>3-2</td><td>2</td></tr>
<tr><td>1</td><td>1</td></tr>
<tr><td>0</td><td>0</td></tr>
</table>

The following table shows how the marks should be awarded for structure and lines of reasoning
<table>
<tr><th></th><th>Number of marks awarded for structure of answer and sustained lines of reasoning</th></tr>
<tr><td>Answer shows a coherent logical structure with linkages and fully sustained lines of reasoning demonstrated throughout</td><td>2</td></tr>
<tr><td>Answer is partially structured with some linkages and lines of reasoning</td><td>1</td></tr>
<tr><td>Answer has no linkages between points and is unstructured</td><td>0</td></tr>
</table>
</td>
<td>
Guidance on how the mark scheme should be applied: The mark for indicative content should be added to the mark for lines of reasoning. For example, a response with four indicative marking points that is partially structured with some linkages and lines of reasoning scores 4 marks (3 marks for indicative content and 1 mark for partial structure and some linkages and lines of reasoning).
If there were no linkages between the points, then the same indicative marking points would yield and overall score of 3 marks (3 marks for indicative content and zero marks for linkages).

In general it would be expected that 5 or 6 indicative points would get 2 reasoning marks, and 3 or 4 indicative points would get 1 mark for reasoning, and 0, 1 or 2 indicative points would score zero marks for reasoning. If there is any incorrect chemistry, deduct mark(s) from the reasoning. If no reasoning mark(s) awarded do not deduct mark(s).

If there is no mention of protons/hydrogens in the response then deduct one structure and reasoning mark
</td>
<td>(6)</td>
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	Indicative content **Similarities** • **IP1**: aromatic hydrogens will give similar/same peaks • **IP2**: both have a peak in the range 1.7-3.0 (ppm) (due to the hydrogen of the H–C–C=O type) **Differences** • **IP3** (Hydrogen environments): Phenylethanone has one less peak/hydrogen environment than phenylethanal • **IP4** (Splitting patterns): a singlet for phenylethanone but a doublet and a triplet in phenylethanal • **IP5** (Peak area ratios): relative peak (area) ratio in phenylethanone is 3 but in phenylethanal the peak (area) ratio is 2 to 1 • **IP6** (Chemical shifts): (Only) phenylethanal has an aldehyde (hydrogen) peak in the range 9 – 10.1 (ppm)	Ignore references to C^{13} nmr Accept annotations on a structure towards crediting the following IPs Allow either a single chemical shift value or a range within the stated values Penalise incorrect chemical shifts Both have peaks in the range 6.5-8.4 (ppm) Ignore any splitting description Ignore any splitting pattern given for this peak to award this mark Allow any difference of one in the number of peaks stated All these splitting patterns required for this IP Ignore the splitting pattern for this IP and ignore any peak areas given for the aryl hydrogens Ignore the splitting pattern for this IP	

Q5.

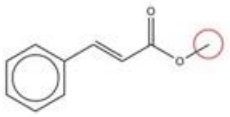
Question Number	Answer	Mark
	The only correct answer is C (6 ..... 7) ***A*** *is not correct because there are six non-equivalent carbons in isoamyl acetate and seven in amyl acetate* ***B*** *is not correct because all carbons of amyl acetate generate their own peak in the spectrum* ***D*** *is not correct because the two methyl groups on the branched chain are equivalent*	**(1)**

Q6.

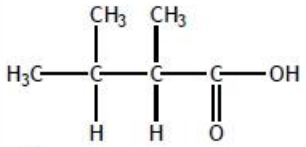
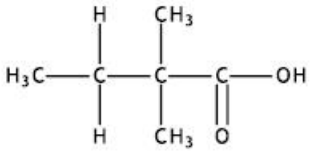
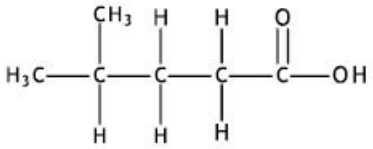
Question Number	Answer	Mark
	The only correct answer is B (6) ***A*** *is not correct because four carbon atoms in the aromatic ring are non-equivalent and not just three, so the correct total of non-equivalent carbon atoms and therefore peaks is six* ***C*** *is not correct because there are two sets of equivalent carbon atoms in the aromatic ring and not just one which means that the correct total of non-equivalent carbon atoms and therefore peaks is six* ***D*** *is not correct because this is the total number of carbon atoms in antifebrin but carbon atoms 2 and 6 in the aromatic ring are equivalent, as are 3 and 5, which gives a correct total of six non-equivalent carbon atoms and therefore six peaks*	**(1)**

Q7.

Question Number	Answer	Additional Guidance	Mark
(i)	An answer that makes reference to the following points: • peak due to tetramethylsilane (1) • so (chemical) shifts (due to other hydrogen atoms) can be compared (1)	 Allow TMS / $Si(CH_3)_4$ Name must be correct if given Allow "a reference" / "a standard" "calibration" Ignore "to allow other molecules to be compared"	(2)

Question Number	Answer	Additional Guidance	Mark
(ii)	An answer that makes reference to the following points: • **M1** circle around $–CH_3$ group in $-OCH_3$ (1) • **M2** singlet as no neighbouring hydrogen atoms (1) • **M3** peak area of 3 means there are 3 hydrogen atoms in this environment (1)	Allow 'protons' for hydrogen atoms  Award whole $-OCH_3$ circled Do not award if C=O included in circle M1 is a stand alone mark Award "has no adjacent hydrogen atoms" Award "no hydrogens on adjacent carbon" Ignore "there is no adjacent C atom" Award "(relative) peak area of three for a $–CH_3$ group" For M3 must relate to (relative) peak area / integral Ignore references to chemical shift value for ester δ = 3.0 to 4.0 (ppm) Ignore references to relative heights of peaks **Comment** M2 and / or M3 dependent on $-CH_3$ group being included in the circled group	(3)

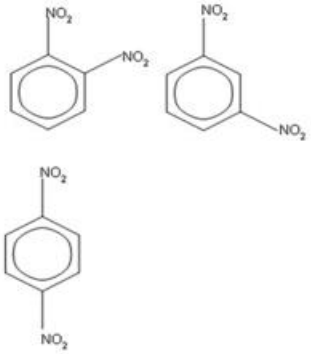
Q8.

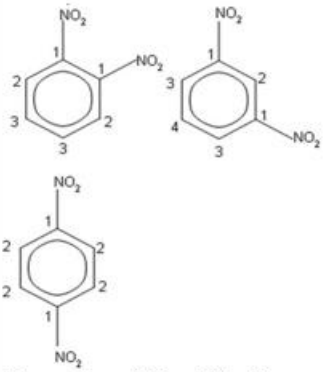
Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	Any two of the following $(CH_3)_2CHCH(CH_3)COOH$ /  **(1)** $CH_3CH_2C(CH_3)_2COOH$ /  **(1)** $(CH_3)_2CHCH_2CH_2COOH$ /  **(1)**	Allow displayed or skeletal formulae	**(2)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)		Do not award other types of structure	**(1)**

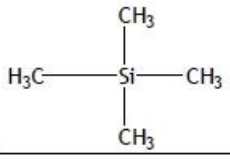
Q9.

Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	$C_6H_4^+$	Allow $H_4C_6^+$ Do not award just C_6H_4	**(1)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)	• 3 correct formulae **(2)**	Examples of formulae  Allow (1) for any 2 correct formulae Allow (2) for three disubstituted benzenes with incorrect substituents / (1) for any two disubstituted benzenes with incorrect substituents Allow incorrectly displayed formulae of NO_2 groups **In (c)(ii) and (iii):** Allow Kekule structures Allow hydrogen atoms shown on benzene Ignore connectivity of NO_2 groups Penalise missing circle in benzene once only	**(2)**

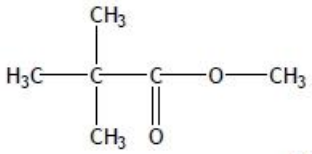
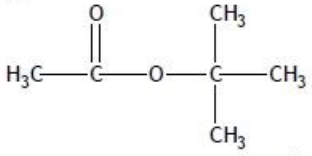
Question Number	Acceptable Answers	Additional Guidance	Mark
(iii)	• **D** identified as 1,3-dinitrobenzene **and** 4 different carbon environments labelled **(1)** • 3 different carbon environments labelled on 1,2-dinitrobenzene **(1)** • 2 different carbon environments labelled on 1,4-dinitrobenzene **(1)**	 Examples of identification These labels may be shown on the structures in (c)(ii) The identification of **D** can be assumed if it is the only structure with 4 carbon environments labelled Allow any form of identification of the carbon environments e.g. numbers, letters, equivalent carbon environments circled TE on disubstituted benzene substituents in (ii) Penalise only half the carbon environments labelled once only	**(3)**

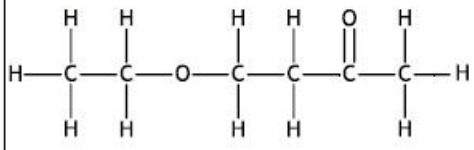
Q10.

Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	$(CH_3)_4Si$	Allow partially or fully displayed formula Ignore connectivity 	**(1)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)	An answer that makes reference to any **two** of the following: • single peak / all H or all C in same environment / no splitting pattern **(1)** • (TMS) peak to the right / upfield / out of the way of other peaks / peak doesn't overlap with other peaks **(1)** • (TMS) low boiling temperature / volatile / can be easily removed **(1)** • gives a strong signal so only a small amount needed **(1)**	Allow 12 H or 4 C in the same environment Ignore references to inertness / non-toxicity / cost / non-polar(ity) Ignore chemical shift = 0 12 H / 4 C are equivalent so gives a strong signal scores 2 marks	**(2)**

Q11.

Question Number	Acceptable Answers	Additional Guidance	Mark
(i)	$C(CH_3)_3COOCH_3$ **or**  **(1)** $CH_3COOC(CH_3)_3$ **or**  **(1)**	Allow displayed or skeletal formulae	**(2)**

Question Number	Acceptable Answers	Additional Guidance	Mark
(ii)	An answer that makes reference to the following points: • the chemical shift δ 2.2 identified **(1)** • four remaining chemical shifts identified **(2)** • two splitting patterns given **and** explained **(2)**	$CH_3C{=}O$ / methyl attached to C=O Identifies 2 or 3 chemical shifts correctly scores 1 δ 1.2 3.5 3.8 2.6 (2.2)  1 specific splitting patterns explained scores 1	(5)

Q12.

Question Number	Answer	Additional Guidance	Mark
	• number of peaks in first product (1) • number of peaks in second product (1)	Number of peaks in the ^{13}C NMR spectrum: 4, 6	(2)

Q13.

Question Number	Answer	Additional Guidance	Mark
(i)	An answer that makes reference to • (**M1**) (similarity) all have arene C–H absorptions Either 3030 (cm^{-1}) **or** 750 and/or 700 (cm^{-1}) **(1)** • (**M2**) only phenol and phenylmethanol have O–H 3750 - 3200 (cm^{-1}) **(1)** • (**M3**) only benzoic acid has O–H 3300 - 2500 (cm^{-1}) **(1)** • (**M4**) only benzoic acid has C=O 1700 - 1680 (cm^{-1}) **(1)** • (**M5**) only phenylmethanol has alkane C–H absorptions either 2962 - 2853 (cm^{-1}) or 1485 - 1365 (cm^{-1}) **(1)**	Bond and wavenumber ranges necessary for each mark Do not award 880/830/780 (cm^{-1}) Do not award –OH / C–OH by penalising once only in M2 and M3 All 5 correct bonds with no wavenumber ranges scores (3) 4 correct etc scores (2) and 3 correct etc scores (1) All 5 correct wavenumber ranges with no bonds or incorrect bonds scores (3) 4 correct etc scores (2) and 3 correct etc scores (1) Penalise any additional peaks once only Ignore references to different fingerprint regions	**(5)**

Question Number	Answer	Additional Guidance	Mark
(ii)	An answer that makes reference to • five peaks (in the ^{13}C NMR spectrum) **(1)** • (four) aromatic peaks within the chemical shift range of 165 - 105 (ppm) **(1)** • (one) peak (for the C-OH) within the chemical shift range of 75 - 55 (ppm) **(1)**	Allow any range within the stated ranges Penalise single values as opposed to ranges once only Accept annotations on diagram Penalise additional peaks once only when three or more types of peak are stated	**(3)**

Question Number	Answer	Additional Guidance	Mark
(iii)	An answer that makes reference to • suitable formula of fragment ion **(1)** • matching *m*/*z* value **(1)**	Example of a suitable formula $C_6H_5COO^+$ or $C_6H_5CO^+$ Do not award $C_7H_5O_2^+$ or $C_7H_5O^+$ *m*/*z* = 121 or 105 Allow $COOH^+$ (1) Do not award bond to the fragment, e.g. $-COOH^+$ *m*/*z* = 45 (1) No TE on incorrect fragment ions such as CH_3^+	**(2)**