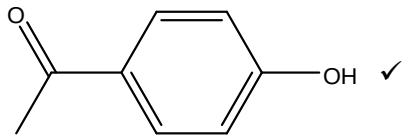


Question	Key	Marks	Guidance
1	C	1	ALLOW 3 (This is the number of peaks in the NMR spectrum)

Question	Answer	Marks	Guidance
2 (a)	Empirical formula Mole Ratio C : H : O = 5.88 : 5.92 : 1.47 ✓ Empirical formula = C₄H₄O ✓ Molecular formula Molecular formula = C₈H₈O₂ AND Evidence of 136 in working or from labelled peak in spectrum ✓	3	ANNOTATE ANSWER WITH TICKS AND CROSSES ALLOW $\frac{70.58}{12.0} : \frac{5.92}{1.0} : \frac{23.50}{16.0}$ ALLOW 4:4:1 if linked to C:H:O Alternative method for 3 marks: C: $\frac{136 \times 70.58/100}{12.0} = 8$ H: $\frac{136 \times 5.92/100}{1.0} = 8$ O: $\frac{136 \times 23.50/100}{16.0} = 2$
(b)	Functional groups Phenol AND ketone ✓ Explanation	3	DO NOT ALLOW any other functional groups for first marking point.

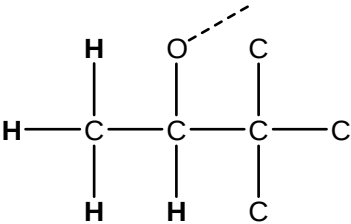
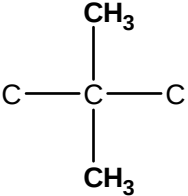
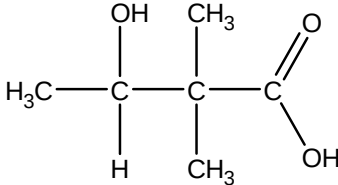
Question			Answer	Marks	Guidance
			Links phenol to (weak) acidity AND no reaction with Na_2CO_3 (so not carboxylic acid) ✓ Links 2,4-DNP(H) or Brady's reagent observation to carbonyl AND Tollens' reagent observation (so not an aldehyde) ✓		ALLOW identity of functional groups in the explanation if not stated on functional group prompt line. ALLOW "aldehyde or ketone" in place of carbonyl
	(c)		Carbon NMR analysis Peaks between 110–160 ppm are the (four) aromatic (carbon environments) ✓ Compound contains a C=O between 190 - 200 ppm AND Compound contains a C-C at 20-30 ppm ✓ Structure 	3	ALLOW peaks to be identified by: • Peaks labelled on spectrum • Peaks indicated on a chemical structure • Peaks indicated from within text Note: If identifying aromatic peaks from the spectrum all four peaks should be indicated. ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous
			Total	9	

Question	Answer	Marks	Guidance
3	A	1	

Question	Answer	Marks	Guidance
4	B	1	ALLOW 4 (This is the number of peaks in the NMR spectrum)

Question		Answer	Marks	Guidance
(a)	5	Number of peaks 2 marks 2-nitrophenol AND 3-nitrophenol have six peaks/environments/types of carbon ✓ 4-nitrophenol has four peaks/environments/types of carbon ✓ Statement 1 mark 4-nitrophenol can be distinguished OR 2-nitrophenol and 3-nitrophenol cannot be distinguished ✓	3	IGNORE any numbers shown on structures ALLOW 1 mark only IF a response identifies that all the compounds have 6 peaks/environments/types of C OR all the compounds have 4 peaks/environments/types of carbon IGNORE chemical shifts DO NOT ALLOW ECF from an incorrect number of peaks/environments/types of carbon

Question	Answer	Marks	Guidance
6*	<i>Please refer to the marking instructions on page 5 of this mark scheme for guidance on how to mark this question.</i> Level 3 (5–6 marks) Compound is a structure of C₆H₁₂O₃ that is consistent with splitting pattern and chemical shifts in NMR spectrum. AND Comprehensive reasoning with most of the data analysed. <i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i> Level 2 (3–4 marks) Compound has a feasible chemical structure that is consistent with the splitting pattern in NMR spectrum but may have incorrect molecular formula. AND Reasoning provided with some of the data analysed. <i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i> Level 1 (1–2 marks) Correct determination of empirical formula and/or molecular formula. OR Analyses most of the NMR data. OR Attempts to determine empirical and/or molecular formula AND analyses some of the NMR data. <i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i>	6	Indicative scientific points: <u>Empirical and Molecular Formula</u> $\begin{array}{rcl} \text{C : H : O} & = & 54.54/12 \quad : \quad 9.10/1 \quad : \quad 36.36/16 \\ & & 4.545 \quad : \quad 9.10 \quad : \quad 2.273 \\ & & 2 \quad : \quad 4 \quad : \quad 1 \end{array}$ - Empirical formula = C₂H₄O - uses $m/z = 132.0$ to determine molecular formula as C₆H₁₂O₃ <u>¹H NMR analysis</u> Spectrum: $\delta = 4.0$ ppm, quartet, 1H, CH₃–CH–O $\delta = 1.3$ ppm, singlet, 6H, (CH₃)₂–C $\delta = 1.2$ ppm, doublet, 3H, CH₃–CH– Without D₂O: - Peak at 11.0 ppm COOH or OH - peak at 3.6 ppm OH Note: Data Sheet shows O–H chemical shift can occur around 11.0 ppm <u>Structure</u> ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous Contains

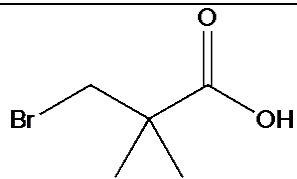
Question	Answer	Marks	Guidance
	0 marks No response or no response worthy of credit.		- region that gives doublet and quartet e.g.  - region that gives singlet e.g.  Examples of structures consistent with splitting and chemical shift in NMR 

Question			Answer	Marks	Guidance
					$\begin{array}{c} \text{OH} \quad \text{O} \quad \text{CH}_3 \\ \quad \quad \\ \text{H}_3\text{C}-\text{C}-\text{C}-\text{C}-\text{OH} \\ \quad \quad \\ \text{H} \quad \quad \text{CH}_3 \end{array}$ $\begin{array}{c} \text{H} \\ \\ \text{H}_3\text{C}-\text{C}=\text{C}-\text{O}-\text{C}-\text{CH}_3 \\ \quad \quad \\ \text{H}_3\text{C} \quad \text{OH} \quad \text{OH} \end{array}$ $\begin{array}{c} \text{CH}_3 \quad \text{OH} \\ \quad \\ \text{H}_3\text{C}-\text{C}-\text{C}-\text{OH} \\ \quad \\ \text{O}-\text{C}-\text{H} \\ \\ \text{CH}_3 \end{array}$ Note: there may be other possible structures that are consistent with the splitting pattern and chemical shifts in NMR – if an alternative structure is seen, please contact your team leader
			Total	18	

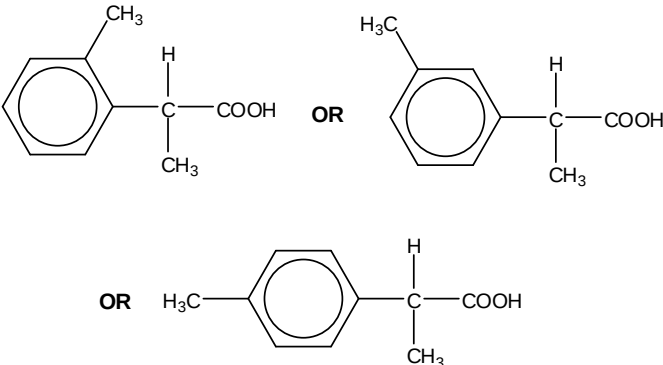
Question	Answer	Marks	AO	Guidance
7	B	1	AO2.5	

Question	Answer	Marks	AO	Guidance
8	C	1	AO2.5	

9	<table><thead><tr><th>Proton environment</th><th>Chemical shift</th><th>Splitting pattern</th></tr></thead><tbody><tr><td>1</td><td>3.0–4.3</td><td>Triplet</td></tr><tr><td>2</td><td>2.0–3.0</td><td>Triplet</td></tr><tr><td>3</td><td>3.0–4.3</td><td>Quartet</td></tr><tr><td>4</td><td>0.5–1.9</td><td>Triplet</td></tr></tbody></table> Mark by column Chemical shift: all 4 correct ✓✓ 3 correct ✓ Splitting pattern: all 4 correct ✓✓ 3 correct ✓	Proton environment	Chemical shift	Splitting pattern	1	3.0–4.3	Triplet	2	2.0–3.0	Triplet	3	3.0–4.3	Quartet	4	0.5–1.9	Triplet	4	AO3.1 × 4	ALLOW δ values ± 0.2 ppm, as a range or a value within the range ALLOW integers for δ values e.g. 2 is equivalent to 2.0 ALLOW quadruplet for quartet ALLOW diagrams to show splitting pattern e.g.  for triplet  for quartet ALLOW splitting patterns shown as numbers i.e. '3' for triplet, '4' for quartet
Proton environment	Chemical shift	Splitting pattern																	
1	3.0–4.3	Triplet																	
2	2.0–3.0	Triplet																	
3	3.0–4.3	Quartet																	
4	0.5–1.9	Triplet																	

Question			Answer	Marks	AO element	Guidance
(c)			 OR 	1	AO3.1	ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous

Question	Answer	Marks	AO element	Guidance
10*	<i>Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question.</i> Level 3 (5–6 marks) Structure is $\text{CH}_3\text{C}_6\text{H}_4\text{CH}(\text{CH}_3)\text{COOH}$ AND Most of the data analysed. <i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i> Level 2 (3–4 marks) A viable aromatic structure of $\text{C}_{10}\text{H}_{12}\text{O}_2$ that contains $\text{C}=\text{O}$ AND most key features consistent with spectral data AND Some of the spectral data analysed <i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i>	6	AO1.2 × 2 AO3.1 × 2 AO3.2 × 2	Indicative scientific points: <u>Empirical and Molecular Formulae</u> $\begin{aligned} \text{C} : \text{H} : \text{O} &= \frac{73.17}{12.0} : \frac{7.32}{1.0} : \frac{19.51}{16.0} \\ &= 6.10 : 7.32 : 1.22 \\ &= 5 : 6 : 1 \end{aligned}$ - Empirical formula = $\text{C}_5\text{H}_6\text{O}$ - uses $m/z = 164.0$ to determine molecular formula as $\text{C}_{10}\text{H}_{12}\text{O}_2$ <u>Structure</u> ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous Key features of an aromatic structure consistent with spectral data - COOH group 4 aromatic H atoms - single H atom that would give a quartet CH_3 group that would give a doublet CH_3 group that would give a singlet

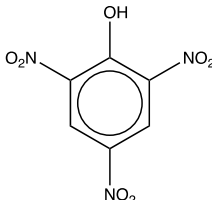
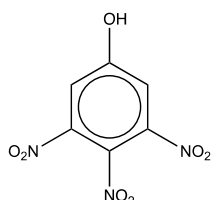
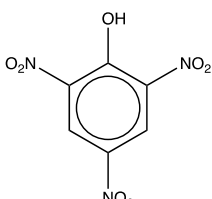
Question	Answer	Marks	AO element	Guidance
	Level 1 (1–2 marks) Correct determination of empirical formula and/or molecular formula. OR Analyses some of the IR and NMR data. OR Analyses most of the NMR data. <i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i> 0 marks No response or no response worthy of credit.			Correct Structure $\text{CH}_3\text{C}_6\text{H}_4\text{CH}(\text{CH}_3)\text{COOH}$ ALLOW 2-, 3- OR 4- substitution of ring <i>i.e.</i>  Spectral analysis ¹H NMR $\delta = 1.6$ ppm, doublet, 3H CH₃–CH– $\delta = 2.3$ ppm, singlet, 3H Ar–CH₃ $\delta = 2.7$ ppm, quartet, 1H CO–CH–CH₃ OR Ar–CH–CH₃ / C₆H₅–CH–CH₃ $\delta = 7.1$–7.5 ppm, multiplet, 4H C₆H₄– ALLOW approximate values for chemical shifts. IR: - peak at 2300–3700 (cm⁻¹) is O–H - peak at ~1720 (cm⁻¹) is C=O - unknown is a carboxylic acid ALLOW ranges from <i>Data Sheet</i> IGNORE references to C–O peaks
	Total	6		

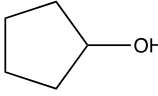
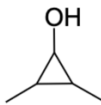
Question	Answer	Marks	AO	Guidance
11	C	1	2.2	

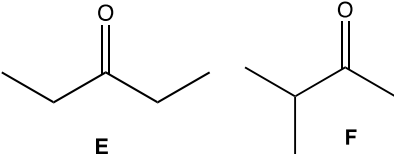
		12					
				Compound C	Compound D		
			Number of peaks	3 ✓	8 ✓		

Question		Answer	Marks	AO element	Guidance
13	(a)	CDCl_3 used as a solvent ✓	2	1.1×2	Example and use required for each mark
		D_2O used to identify OH OR NH protons ✓			ALLOW for 1 mark, D_2O as a solvent

Question	Answer	Marks	AO element	Guidance
14	B	1	AO2.1	

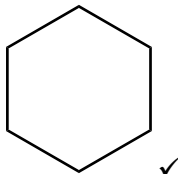
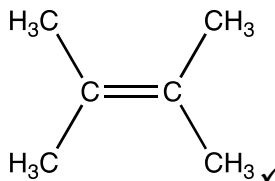
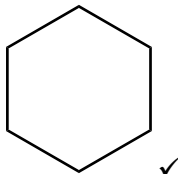
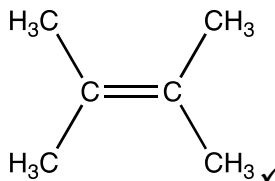
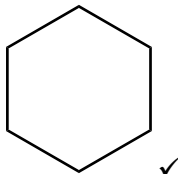
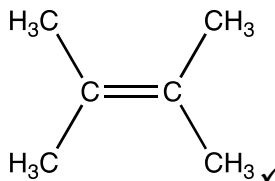
						DO NOT ALLOW adding of a drying agent (e.g. MgSO ₄)
	15	C : H : N : O 31.44/12 : 1.31/1 : 18.34/14 : 48.91/16 OR 2.62 : 1.31 : 1.31 : 3.06 ✓ 6:3:3:7 OR C₆H₃N₃O₇ ✓ Molecular formula = C₆H₃N₃O₇ AND use of <i>M</i> = 229.0 (directly linked to molecular formula) ✓ Any trisubstituted –NO₂ substituted phenol that is consistent with <i>M</i> = 229.0 ✓ Evidence for substitution 2,4,6 OR 3,4,5 substituted phenol AND 4 peaks/ C environments from ¹³C NMR ✓ 2,4,6 substituted phenol AND directing effects of –OH ✓	6	AO1.2 × 2 AO3.1 AO3.2 AO3.1 ×2  2,4,6  3,4,5  2,4,6	ALLOW alternative approach for empirical formula and evidence that 229 is equal to C₆H₃N₃O₇ DO NOT ALLOW ECF from the empirical formula with the wrong molar ratio	

Question	Answer	Marks	AO element	Guidance
16*	<i>Refer to marking instructions on page 5 of mark scheme for guidance on marking this question.</i> Level 3 (5–6 marks) Compounds D, E AND F correctly identified AND Most of the observations and NMR data analysed. <i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i> Level 2 (3–4 marks) Most of compounds D, E AND F correctly identified AND Some of the observations and NMR data analysed. <i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i> Level 1 (1–2 marks) Most of compounds D, E AND F correctly identified OR Some of compounds D, E AND F correctly identified AND Analyses some of the observations or NMR data OR Analyses most of the observations from the test-tube tests. OR Analyses most of the NMR data. OR Analyses some of the observations and NMR data	6	AO3.1 ×4 AO3.2 ×2	Indicative scientific points may include: <u>Observations from Test-tube tests</u> 2,4 DNP D has no C=O E and F have C=O present $\text{H}^+/\text{Cr}_2\text{O}_7^{2-}$ D is primary OR secondary alcohol E and F are ketones (<i>negative test shows not aldehydes</i>) Br_2 D, E and F have no C=C/are saturated ¹³C NMR analysis D: • 3 carbon environments/types of C • $\delta = 24, 36 \text{ ppm}$ C–C • $\delta = 73 \text{ ppm}$, C–O ¹H NMR analysis E: • $\delta = 2.4 \text{ ppm}$, quartet $\text{CH}_3\text{--CH}_2\text{--C=O}$ • $\delta = 1.1 \text{ ppm}$, triplet $\text{CH}_3\text{--CH}_2\text{--}$ F: • $\delta = 2.6 \text{ ppm}$, heptet/multiplet $(\text{CH}_3)_2\text{--CH--C=O}$ • $\delta = 2.1 \text{ ppm}$, singlet, $\text{CH}_3\text{--C=O}$ • $\delta = 1.1 \text{ ppm}$, doublet $\text{CH}_3\text{--CH--}$ <u>Structures</u> ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous  D OR 

Question			Answer	Marks	AO element	Guidance
			<i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i> 0 marks No response or no response worthy of credit.			 E F
			Total	6		

Question	Answer	Marks	AO	Guidance
17	A	1	AO2.1	

Question	Answer	Marks	AO	Guidance
18	B	1	AO2.1	

Question			Answer	Marks	element	Guidance				
16	(b)	19	<table border="1"><tr><td></td><td></td></tr><tr><td>D</td><td>E</td></tr></table> Two of the following for D ✓ • All H are equivalent/in the same chemical environment/ the same type • All C are equivalent/ in the same chemical environment/ the same type • No C=C present Two of the following for E ✓ • All H are equivalent/ in the same chemical environment/ the same type • 2 C environments • C=C present			D	E	4	AO2.5 ×2 AO2.2 ×2	ALLOW 1 mark for structures if shown in wrong boxes. CHECK table 16.1 for annotations that may be worthy of credit
										
D	E									

[illegible]

						(Add) FeCl ₃ AND violet/purple colour ✓
20	(a)	21	Compound J has 6 peaks/environments/types of carbon ✓ Compound K has 5 peaks/environments/types of carbon ✓ Compound L has 8 peaks/environments/types of carbon ✓	3	AO3.2 ×3	IGNORE any numbers shown on structures IGNORE chemical shifts

Question	Answer	Marks		Guidance
22	C	1	AO1.1	

Question	Answer	Marks		Guidance
23	C	1	AO2.1	

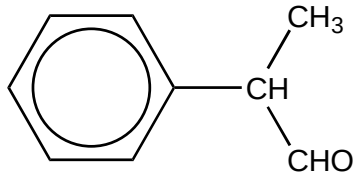
Question		Answer	Marks	element	Guidance
17	24	Structures 1 mark $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ AND $\text{CH}_3\text{CH}_2\text{CHOHCH}_3$ AND $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$ AND $(\text{CH}_3)_3\text{COH}$ ✓ Number of peaks 3 marks $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$/ butan-1-ol OR $\text{CH}_3\text{CH}_2\text{CHOHCH}_3$/ Butan-2-ol have 4 peaks/environments/types of carbon ✓ $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$/ (2-)methylpropan-1-ol has 3 peaks/environments/types of carbon ✓ $(\text{CH}_3)_3\text{COH}$/(2-)methylpropan-2-ol has 2 peaks/environments/types of carbon ✓ Statement 1 mark $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$/(2-)methylpropan-1-ol can be distinguished (from any other isomer) OR $(\text{CH}_3)_3\text{COH}$/(2-)methylpropan-2-ol can be distinguished (from any other isomer) OR $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$/ butan-1-ol AND $\text{CH}_3\text{CH}_2\text{CHOHCH}_3$/ butan-2-ol cannot be distinguished ✓	5	AO2.1 AO3.1 ×3 AO3.2 ×1	ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous Note: all 4 structures are needed for the mark. Additional incorrect structures prevent this mark being awarded. IGNORE chemical shifts IGNORE incorrect name if structure given ALLOW correct number of peaks linked to an incomplete structure e.g. C-C-C-C-OH has 4 peaks (no hydrogens shown) Statement mark can only be awarded if candidate compares at least two isomers and determines correct number of peaks for the isomers referred to. DO NOT ALLOW ECF from an incorrect number of peaks/environments/types of carbon

Question	Answer	Marks	AO element	Guidance
25	<i>Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question.</i> Level 3 (5–6 marks) Structure is either $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{C}(\text{CH}_3)_3$ OR $(\text{CH}_3)_3\text{CCH}_2\text{COOCH}_2\text{CH}_3$ AND Most of the data analysed. <i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i> Level 2 (3–4 marks) Structure is an ester of $\text{C}_8\text{H}_{16}\text{O}_2$ with some key features present AND Analyses some of the data from at least 3 of the scientific points. <i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i> Level 1 (1–2 marks) Attempts analysis from at least 2 of the scientific points. <i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i> 0 marks No response or no response worthy of credit.	6	AO1.2 × 2 AO3.1 × 2 AO3.2 × 2	Mark spectra page as SEEN Indicative scientific points: 1. Empirical Formulae $\begin{aligned} \text{C} : \text{H} : \text{O} &= \frac{66.63}{12.0} : \frac{11.18}{1.0} : \frac{22.19}{16.0} \\ &= 5.55 : 11.18 : 1.39 \\ &= 4 : 8 : 1 \end{aligned}$ - Empirical formula = $\text{C}_4\text{H}_8\text{O}$ 2. Molecular Formulae - uses $m/z = 144.0$ to determine molecular formula as $\text{C}_8\text{H}_{16}\text{O}_2$ 3. Functional group From IR, → $\text{C}=\text{O}$ from $\sim 1740 \text{ cm}^{-1}$ IGNORE references to $\text{C}-\text{O}$ peaks No reaction with 2,4-DNP → no carbonyl/no ketone and aldehyde - Likely to be an ester 4. ^1H NMR analysis $\delta = 0.9 \text{ ppm}$, singlet, 9H $-\text{C}(\text{CH}_3)_3$ $\delta = 1.2 \text{ ppm}$, triplet, 3H CH_3CH_2- $\delta = 2.2 \text{ ppm}$, quartet, 2H $\text{CH}_3\text{CH}_2\text{CO}$ $\delta = 4.1 \text{ ppm}$, singlet, 2H $-\text{OCH}_2-$ ALLOW approximate values for chemical shifts.

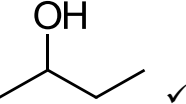
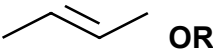
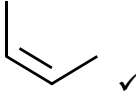
Question	Answer	Marks	AO element	Guidance
				Structure ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous Key features consistent with chemical shift data and relative peak areas • O-CH₂ • C(CH₃)₃ • CH₃CH₂C=O Correct Structure • CH₃CH₂COOCH₂C(CH₃)₃ O CH₃

Question	Answer	Marks	Guidance
26	B	1	

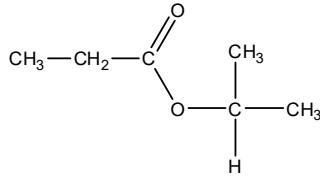
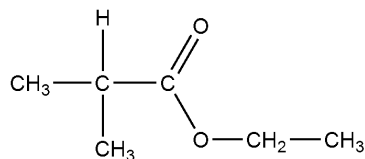
Question	Answer	Marks	Guidance
27*	Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question. Level 3 (5–6 marks) Structure is $\text{C}_6\text{H}_5\text{CHCH}_3\text{CHO}$ AND Analyses data from all 3 scientific points <i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i> Level 2 (3–4 marks) Structure with most key features including O atom(s) AND Analyses data from at least 2 of the scientific points <i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i> Level 1 (1–2 marks) Attempts analysis from at least 2 of the scientific points <i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i> 0 marks No response or no response worthy of credit.	6	LOOK ON THE SPECTRA for labelled peaks and mark as SEEN Indicative scientific points: <u>1. Empirical (and Molecular) Formulae</u> $\begin{aligned} \text{C} : \text{H} : \text{O} &= \frac{80.60}{12.0} : \frac{7.46}{1.0} : \frac{11.94}{16.0} \\ &= 6.72 : 7.46 : 0.746 \\ &= 9 : 10 : 1 \end{aligned}$ - Empirical formula = $\text{C}_9\text{H}_{10}\text{O}$ <u>2. Mass spectrum and IR</u> Mass spectrum - uses $m/z = 134$ to give molecular formula: $\text{C}_9\text{H}_{10}\text{O}$ - Any possible fragments: $m/z = 105$ $\text{C}_6\text{H}_5\text{CHCH}_3^+$ $m/z = 77$ C_6H_5^+ $m/z = 29$ CHO^+ IR $\text{C}=\text{O}$ from $\sim 1700\text{ cm}^{-1}$ - Likely to be aldehyde or ketone $\text{C}=\text{C}$ (arenes) $\sim 1500\text{ cm}^{-1}$ ALLOW Data Sheet ranges <u>3. ^1H NMR</u> $\delta = 1.4$ ppm, doublet, 3H $\text{CH}_3\text{CH}-$ $\delta = 3.8$ ppm, quintet, 1H next to 4 adjacent H $\delta = 7.3$ ppm, singlet, 5H C_6H_5- $\delta = 9.0$ ppm, doublet, 1H $-\text{CHCHO}$ ALLOW approximate values for chemical shifts

		Structure ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous ALLOW correct Kekulé representation of benzene Key features • Benzene ring • C=O • CH₃ Correct structure  • (C₆H₅CHCH₃CHO) Aspects of the communication statement being met might typically include: • Structures given are feasible and unambiguous • Easy to follow layout on empirical formula calculation • Empirical formula is shown to be same as molecular • IR peaks linked clearly to bond it refers to not just functional groups • Positive charge given on MS fragments • MS fragments plausible for the molecular formula determined • Clear information for each NMR peak • No additional irrelevant/incorrect information given
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Question	Answer	Marks	Guidance
28	D	1	

Question	Answer	Mark	Guidance
29 (a)	Functional group and reasoning for compound K alcohol AND OH AND peak at 3200 – 3600 (cm⁻¹) ✓ Possible structures of K, L and M K =  ✓ L =  ✓ M =  OR  ✓	4	DO NOT ALLOW any other functional group e.g. phenol, carboxylic acid IGNORE 'hydroxyl' for 'alcohol' BUT ALLOW for O-H ALLOW any stated value in range 3100 to 3600 (cm⁻¹) <i>(consistent with spectrum provided)</i> IGNORE reference to C-O If no or incomplete answer, check spectrum for annotations – credit can be given from a correctly labelled peak (values are not needed) ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous ALLOW one mark if L and M both correct but in the wrong boxes

Question	Answer	Mark	Guidance
29 (b)*	<i>Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question.</i> Level 3 (5–6 marks) Structure is either $\text{CH}_3\text{CH}_2\text{COOCH}(\text{CH}_3)_2$ OR $(\text{CH}_3)_2\text{CHCOOCH}_2\text{CH}_3$ AND Most of the data analysed <i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i> Level 2 (3–4 marks) Structure has a molecular formula of $\text{C}_6\text{H}_{12}\text{O}_2$ with at least two key features present AND Analyses some of the data from the NMR <i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i> Level 1 (1–2 marks) Attempts analysis from at least 2 of the scientific points. <i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i> 0 marks No response or no response worthy of credit.	6	Mark spectra page as SEEN Indicative scientific points: 1. Empirical Formula $\text{C} : \text{H} : \text{O} = \frac{62.07}{12.0} : \frac{10.34}{1.0} : \frac{27.59}{16.0}$ $= 5.17 : 10.34 : 1.72$ $= 3 : 6 : 1$ - Empirical formula = $\text{C}_3\text{H}_6\text{O}$ ALLOW Alternative method using Mr of 116 e.g $(0.6270 \times 116) \div 12 = 6$ 2. Molecular Formula and Mass Spectrum - uses $m/z = 116.0$ to determine molecular formula as $\text{C}_6\text{H}_{12}\text{O}_2$ - Any possible fragments, for example: $m/z = 43$ $(\text{CH}_3)_2\text{CH}^+$ $m/z = 29$ CH_3CH_2^+ 3. ^1H NMR analysis $\delta = 1.1$ ppm, triplet, 3H CH_3CH_2- $\delta = 1.4$ ppm, doublet, 6 H $-\text{CH}(\text{CH}_3)_2$ $\delta = 2.4$ ppm, quartet, 2H $\text{CH}_3\text{CH}_2\text{CO}$ $\delta = 4.4$ ppm, heptet, 1H $-\text{OCH}(\text{CH}_3)_2$ ALLOW approximate values for chemical shifts. ALLOW multiplet for heptet 4. Structure ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous

Question			Answer	Mark	Guidance
					Key Features • Carbonyl -C=O • C-O bond • Ethyl group -CH₂CH₃ • Dimethyl group -C(CH₃)₂ Correct structure  Justified from NMR chemical shift analysis OR  Justified from MS fragment as (CH₃)₂CHCO⁺ at 71 Aspects of the communication statement being met might typically includes; • Structures given are feasible and unambiguous • Justifying the correct structure from the evidence • Easy to follow layout on empirical formula calculation • Plausible MS fragments (ideally with a positive charge shown) • Clear information for each NMR peak, including use of correct terminology for splitting patterns • No additional irrelevant/incorrect information given