Mark scheme

Question	Answer/Indicative content	Marks	Guidance
1	*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 $C_6H_5CHCH_3CHO$ **AND** Analyses data from **all 3** scientific points *There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.* **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 *There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.* **Level 1 (1-2 marks)** Attempts analysis from **at least 2** of the scientific points *There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.* **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:** **1. Empirical (and Molecular) Formulae** • $C:H:O = \frac{80.60}{12.0} : \frac{7.46}{1.0} : \frac{11.94}{16.0}$ $= 6.72 : 7.46 : 0.746$ $= 9 : 10 : 1$ • Empirical formula = $C_9H_{10}O$ **2. Mass spectrum and IR** **Mass spectrum** • uses *m*/*z* = 134 to give molecular formula: $C_9H_{10}O$ • Any possible fragments: - m/z = 105 $C_6H_5CHCH_3^+$ - m/z = 77 $C_6H_5^+$ - m/z = 29 CHO^+ **IR** • C=O from ~1700 cm^{-1} • Likely to be aldehyde or ketone • C=C (arenes) ~1500 cm^{-1} **ALLOW** *Data Sheet ranges* **3. ^{1}H NMR** • δ = 1.4 ppm, doublet, 3H **CH_3**CH− • δ = 3.8 ppm, quintet, 1H next to 4 adjacent H • δ = 7.3 ppm, singlet, 5H **$C_6H_5^-$** • δ = 9.0 ppm, doublet, 1H -CH**CHO** **ALLOW** approximate values for chemical

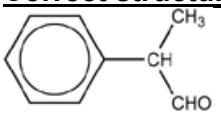
shifts

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
- CH_3

Correct structure



- ($C_6H_5CHCH_3CHO$)

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

Examiner's Comments

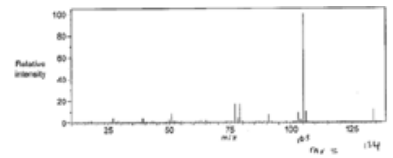
This question was well-attempted by most candidates, with the majority of candidates gaining full marks or gaining 4 marks for a top Level 2 response.

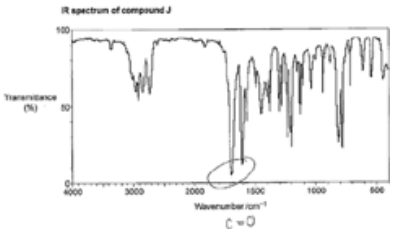
					Many candidates showed excellent recall of how to determine the correct empirical formula from the percentage composition data. Most then went on to use the m/z peak on the mass spectrum to confirm that the M_r was 134, and therefore the molecular formula was identical to the empirical formula. A few also made use of the mass spectrum to identify possible fragment ions including a correct positive charge. Most candidates used the IR spectrum to identify a C=O bond and many also mentioned the absence of O-H or spotted C=C for arenes. Lower attaining candidates sometimes incorrectly mentioned the presence of a carboxylic acid O-H despite the molecular formula only having 1 oxygen atom. Many candidates annotated the NMR spectrum and/or presented their analysis clearly in a table format and were able to identify aldehyde and arene hydrogen environments. The best candidates hadfragments built up alongside their NMR analysis clearly building them using chemical shift, integratio ratios and splitting patterns. Those that struggled to interpret the splitting patterns correctly suggested incorrect structures but often with correct features so were still able to score Level 2, 4 marks. Some initially identified the multiplet peak at3.8ppm as being **H**C-O environment but many realised this did not fit the IR data. However, some changed other evidence to fit this, e.g. the peak at 9.0 ppm being an O-**H** rather than C**H**O and the IR having C=C only without C=O as well. A large proportion of candidates were able to correctly determine the structure of compound **J**, recognising that the peak at 3.8 ppm was shifted up-field as adjacent to both the benzene ring and the aldehyde group. The data sheet refers to this: 'C**H** bonded to 'shifting groups' on either side, e.g. $O-CH_2-C=O$, may be shifted more than indicated above'. Several candidates who did not get the correct structure gave structures which were chemically unfeasible, e.g. with pentavalent carbons. Many candidates had several structures as part of working but did not

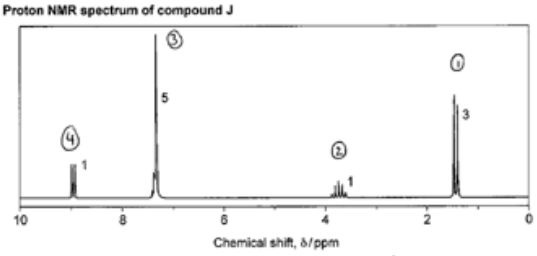
always ensure their final structure was clearly highlighted.

A very small number of candidates received no credit for this question, as the majority were able to show analysis of 2 aspects, e.g. the calculation of empirical formula and labelling of IR or NMR spectra.

Exemplar 3







The numbers by the peaks are the relative peak areas.

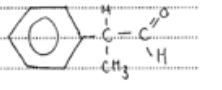
Determine the structure of compound J, showing **all** your reasoning. **[6]**

elemental analysis:

$n(C) = \frac{80.60}{12} = \frac{6.71667}{0.74625} = 9$

$n(H) = \frac{7.46}{1} = \frac{7.46}{0.74625} = 10$ $C_9H_{10}O = 134$

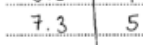
$n(O) = \frac{11.94}{16} = \frac{0.74625}{0.74625} = 1$

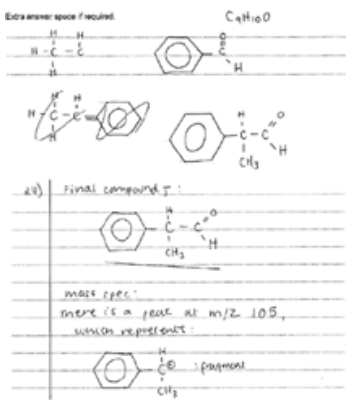


Infrared:

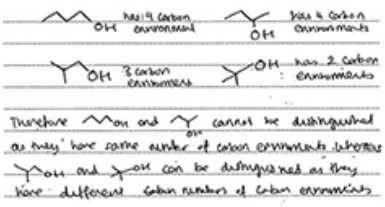
→ There is a peak at 1700 cm^{-1}, which represents C=O bond, which occurs between 1630-1820 cm^{-1} by aldehyde or ketone.

H' NMR:

	/ppm/δ	n.o of hydrogen	splitting	n.o of H on adjacent	
①	1.5	3	doublet	1	H_3C-CH
②	3.8	1	multiplet	4	$HC-CH_3$
③	7.3	5	doublet singlet	01	
④	9.0	1	doublet	1	$-C(=O)H$ (aldehyde)

					 Level 3, 6 marks There is clear and detailed analysis throughout this response to determine the correct final structure for **J**. The empirical formula calculation shows how the empirical formula was determined. On the mass spectrum the annotation links to the M_r of 134 and at the end of the response they have identified the fragment responsible for the parent ion. The C=O IR peak is labelled and described in the response. The NMR analysis is clear, with each peak being numbered and linked to a table which shows how the candidate has identified the hydrogens responsible for each peak as well as linking to neighbouring hydrogens from splitting patterns. The final compound is labelled as such to distinguish it clearly from other structures given, which were part of their problem solving to find a structure that fits all of the analysis they had completed.
			Total	**6**	
2			**D**	1	**<u>Examiner's Comments</u>** Many missed the separate O–H in alcohol and O–H in carboxylic acid peaks as it is unusual to see clearly defined peaks for both in an IR spectrum. Those who got D tended to annotate the spectrum, noting the sharp peak as O–H bond, as well as drawing out structures for each option. A was the most common incorrect response. It is good to remind candidates to look at all possible options before making a final decision.
			Total	**1**	

3			**B**	1	**Examiner's Comments** Around two-thirds picked the correct answer B, identifying Structures 1 and 2 as having 2 carbon environments. Most students labelled the carbon environments on the structures to help them. Candidates sometimes struggled to recognise the two different carbon environments within the benzene ring, in Structure 3, as well as the CH_3 group.
			Total	**1**	
4			**Structures 1 mark** $CH_3CH_2CH_2CH_2OH$ **AND** $CH_3CH_2CHOHCH_3$ **AND** $(CH3)_2CHCH_2OH$ **AND** $(CH_3)_3COH$ ✓ **Number of peaks 3 marks** $CH_3CH_2CH_2CH_2OH$/ butan-1-ol **OR** $CH_3CH_2CHOHCH_3$ / Butan-2-ol have 4 peaks/environments/types of carbon ✓ $(CH_3)_2CHCH_2OH$/ (2-)methylpropan-1-ol has 3 peaks/environments/types of carbon ✓ $(CH_3)_3COH$/(2-)methylpropan-2-ol has 2 peaks/environments/types of carbon ✓ **Statement 1 mark** $(CH_3)_2CHCH_2OH$/ (2-)methylpropan-1-ol can be distinguished (from any other isomer) **OR** $(CH_3)_3COH$/(2-)methylpropan-2-ol can be distinguished (from any other isomer) **OR** $CH_3CH_2CH_2CH_2OH$/ butan-1-ol **AND**	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 **Examiner's Comments** This question discriminated well with a variety of responses seen. The lower scoring candidates gave vague answers suggesting they did not fully grasp what the question was asking. They often filled the lines with generic responses in terms of what C NMR can do, e.g. chemical shift data/shows positions of Cs relative to OH group or number of peaks gives number of environment but made no

			$CH_3CH_2CHOHCH_3$/ butan-2-ol cannot be distinguished ✓		reference to the isomers mentioned in the question. For some there was obvious confusion with proton NMR due to discussion of splitting patterns or relative peak areas/heights. Lots struggled to find all four isomers, often repeating one they already had, but drawing them with a different layout, or by giving cyclic structures. Some struggled to count the correct number of peaks for each. It was common to see false equivalency between CH_2 groups, e.g. butan-2-ol with three peaks. Many struggled to give a concluding statement, often focusing more on slight differences in chemical shift due to proximity to OH group. The highest scoring responses were well structured and started by identifying the four isomers. After stating the number of carbon environments for each isomer these responses often concluded with a statement detailing whether the isomers could be distinguished. **Assessment for learning** Candidates often struggle with drawing out the different structural isomers. As a starter activity or plenary give candidates a molecular formula and challenge them to draw out all the different possible isomers. Using molymod can help candidates realise equivalent molecules. As candidates become more confident encourage them to draw structures using skeletal formula and to give the systematic names. Exemplar 2  This candidate has clearly drawn out all four isomer structures and next to each has identified the number of carbon environments.

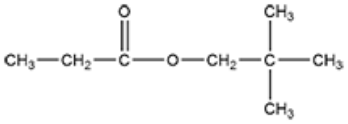
					They have then made a concluding statement using this information. This response scored all 5 marks.
			Total	**5**	
5			**Level 3 (5–6 marks)** Structure is either $CH_3CH_2COOCH_2C(CH_3)_3$ **OR** $(CH_3)_3CCH_2COOCH_2CH_3$ **AND** Most of the data analysed. *There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.* **Level 2 (3–4 marks)** Structure is an ester of $C_8H_{16}O_2$ with **some** key features present **AND** Analyses some of the data from at least 3 of the scientific points. *There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.* **Level 1 (1–2 marks)** Attempts analysis from at least 2 of the scientific points. *There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.* **0 mark** 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** • C : H : 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 • Empirical formula = C_4H_8O **2. Molecular Formulae** • uses *m/z* = 144.0 to determine molecular formula as $C_8H_{16}O_2$ **3. Functional group** From IR, • → C=O from ~1740 cm^{-1} **IGNORE** references to C–O peaks No reaction with 2,4-DNP • → no carbonyl/no ketone and aldehyde • Likely to be an ester **4.** ^1H NMR analysis • δ = 0.9 ppm, singlet, 9H –C**$(CH_3)_3$** • δ = 1.2 ppm, triplet, 3H **CH_3**CH_2– • δ = 2.2 ppm, quartet, 2H CH_3**CH_2**CO • δ = 4.1 ppm, singlet, 2H –**OCH_2**– **ALLOW** approximate values for chemical shifts. **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-CH_2
- $C(CH_3)_3$
- $CH_3CH_2C{=}O$

Correct Structure

- $CH_3CH_2COOCH_2C(CH_3)_3$



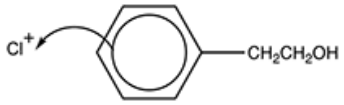
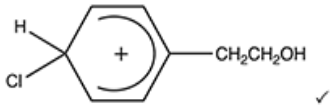
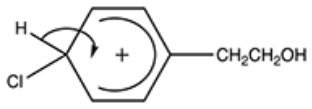
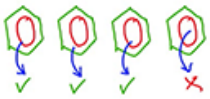
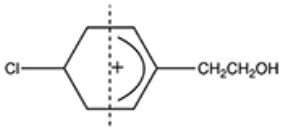
Examiner's Comments

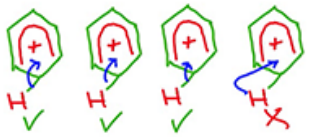
Most candidates were able to deduce the empirical and/or molecular formula of the organic compound. Analysis of the IR spectrum was also well attempted, but some candidates assumed the unknown was a carboxylic acid, attributing the sharp peak just below 3000 cm^{-1} to an OH group. Others misidentified the C=O peak as a C=C group suggesting alkene or arene structure. They were often led to this conclusion as they believed no precipitate with 2,4-DNP suggested no C=O rather than no aldehyde or ketone.

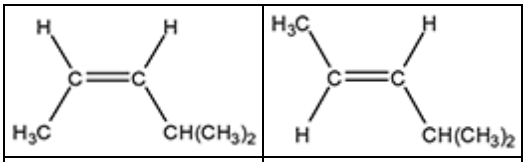
Good analysis of the NMR data was crucial for deducing the correct ester. Some candidates opted to annotate the proton NMR spectrum, some produced tables and others gave written details for each peak. It was vital that they were able to interpret all information for each peak i.e. number of proton environments, the type of environment from chemical shift, the number of protons in each environment from relative peak areas and use of splitting patterns to find information about adjacent protons. Many tried to make the data fit their proposed structure rather than the other way round. Some suggested structures that were only partially consistent with the data such as

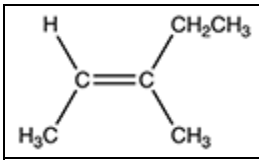
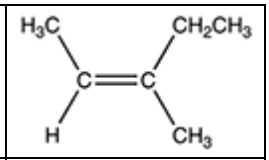
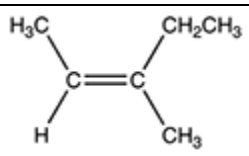
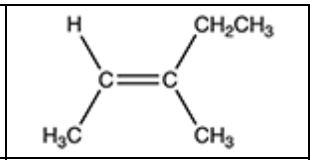
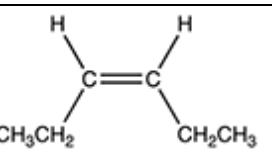
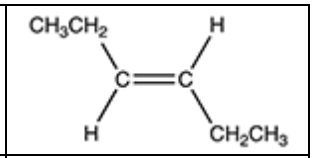
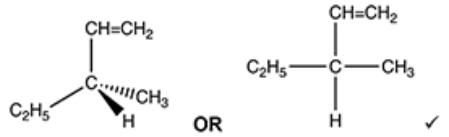
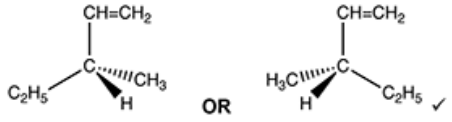
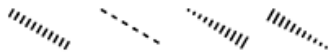
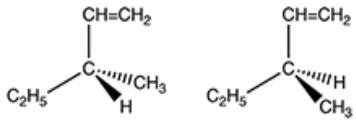
					$CH_3CH_2CH_2COOC(CH_3)_3$ and were awarded Level 2. Others did not take full note of all the information provided, for example omitting the 2,4-DNP observations, giving the ketone $(CH_3)_3COCH_2COCH_2CH_3$ or not checking it matched the molecular formula $CH_3CH_2COOC(CH_3)_3$ so only achieved Level 1. Candidates need to be encouraged to draw a structure as without they can only achieve a maximum of 2 marks despite some excellent analysis of the data. Conversely, it is not sufficient to just give a structure, candidates must give analysis of the data provided. Exemplar 3  This is a good Level 3 6 mark response. As well as this clearly laid out analysis they also had details written on the question, e.g. no aldehyde or ketone due to no reaction with 2,4-DNP. This response has been selected due to the detailed analysis of NMR data that has been summarised in a table.
			Total	**6**	
6			**C**	1 (AO2.1)	**<u>Examiner's Comments</u>** Many candidates wrote the number of proton environments next to each structure, circling or marking protons, but some struggled to

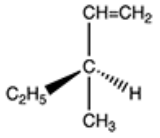
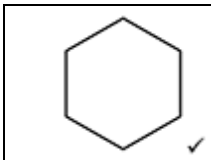
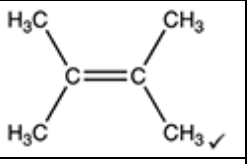
					spot equivalent environments in the skeletal structures. A and D were common incorrect responses. The correct answer also included -OH protons which candidates did not always include in their count.
			Total	**1**	
7			**C**	1 (AO1.1)	**Examiner's Comments** Many candidates were not able to identify the compound used for proton exchange, D_2O (C) and instead selected either $CDCl_3$ (B), a common NMR solvent, or TMS (D), an NMR standard. Potentially candidates may be familiar with shaking with D_2O to remove -OH and -NH protons but may not realise this is known as 'proton exchange'.
			Total	**1**	
8		i	Indicator **AND** observation of acidity **AND** No reaction with carbonate ✓	1 (AO1.2×1)	**ALLOW** (Add) bromine **AND** white precipitate ✓ **ALLOW** (Add) $FeCl_3$ **AND** violet/purple colour ✓
		ii	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
		iii	**ANNOTATE ANSWER WITH TICKS AND CROSSES** **Action of catalyst 1 mark** Formation of electrophile: $Cl_2 + AlCl_3 \rightarrow$	4 (AO1.2×2) (AO2.5×2)	**ALLOW** use of $FeCl_3$ or other halogen carriers

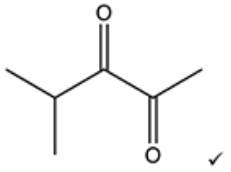
			$Cl^+ + AlCl_4^-$ **AND** Regeneration of catalyst: $H^+ + AlCl_4^- \rightarrow AlCl_3 + HCl$ ✓ **----------** **Electrophilic attack 1 mark** Curly arrow from π-bond to Cl^+ ✓  **Correct intermediate only 1 mark**  ✓ **----------** **Reforming benzene ring 1 mark** Curly arrow from C–H bond to reform π-ring ✓  		($AlBr_3$) **----------** **For curly arrows, ALLOW straight or snake-like arrows and small gaps (see examples):** **----------** **1st curly arrow** must • start from, **OR** close to **circle of benzene ring** **AND** • go to Cl^+  **DO NOT ALLOW** the following intermediate:  π-ring must cover more than half of benzene ring **AND** correct orientation, *i.e.* gap towards C with Cl **ALLOW** + sign anywhere inside the 'hexagon' of intermediate **DO NOT ALLOW** intermediates substituted at positions 3 or 5 **IGNORE** intermediates substituted at position 2 **OR** di-substituted at positions 2,4 **----------** **Curly arrow** must start from, **OR** be traced back to, **any part of** C–H bond and go inside the 'hexagon'

					 **Examiner's Comments** Few candidates knew the test for a phenol group. Frequent incorrect responses involved the production of a gas with a carbonate or stating that bromine water is decolourised but failing to state that a white precipitate is also formed. A significant number of candidates also stated that the reaction with sodium hydroxide confirms the presence of the phenol group. This question proved challenging to candidates with few scoring all 3 marks. Where no marks were given, this was frequently because candidates did not state the number of carbon environments in compounds J, K and L. Candidates who were given 1 or two marks frequently stated the incorrect number of peaks that would be observed. This question required candidates to apply their knowledge of the mechanism of electrophilic substitution. Examiners were encouraged by the number of excellent responses to this question, with the majority of candidates securing 3 out of 4 marks. Common errors included the omission of HCl as product from the regeneration of the catalyst or candidates attempting to substitute at the 2 position.
			Total	**8**	
9			A	1 (AO2.1)	**Examiner's Comments** This question proved challenging. Candidates who drew out the different compounds were able to identify A as the correct response.
			Total	**1**	
10			B	1 (AO2.1)	

					Examiner's Comments Candidates found this question difficult. Those who drew out the different compounds were able to identify B as the correct response.
			Total	**1**	
11		i	Same **molecular** formula **AND** Different **structural** formulae ✓ **OR** Both have the **molecular** formula C_6H_{12} **AND** Different **structural** formulae ✓	1 (AO1.1)	Same formula is **not** sufficient *(no reference to molecular)* Different arrangement of atoms is **not** sufficient *(no reference to structure/structural)* For 'structural formulae', **ALLOW** structure/displayed/skeletal formulae/functional groups **DO NOT ALLOW** any reference to spatial/space
		ii	Same structural formula **AND** Different arrangement (of atoms) in **space** **OR** different **spatial** arrangement (of atoms) ✓	1 (AO1.1)	**ALLOW** structure/displayed/skeletal formula **DO NOT ALLOW** same empirical formula **OR** same general formula **IGNORE** same molecular formula Reference to *E/Z* isomerism or optical isomerism is **not** sufficient
		iii	Correct identification of *cis* **AND** *trans* isomers of 4-methylpent-2-ene ✓✓  *cis* isomer | *trans* isomer **OR** Identification of 3-methylpent-2-ene as *cis* **AND** *trans* isomers ✓✓	2 (AO1.2) (AO2.5)	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous C_3H_7 is **not** sufficient (could be unbranched) **ALLOW** one mark if *cis* **AND** *trans* isomers of 4-methylpent-2-ene are in the wrong boxes **ALLOW** the isomers of 3-methylpent-2-ene in either box

			 *cis* isomer  *trans* isomer		 *cis* isomer  *trans* isomer *Ambiguity with cis/trans identification system* **ALLOW** one mark for correct identification of *cis* **AND** *trans* isomers of unbranched C_6H_{12} e.g.  *cis* isomer  *trans* isomer
		iv	Correct groups attached to chiral carbon of compound C seen **once** e.g.  ✓ Two **3D structures** of compound C that are mirror images with correct connectivity in both  ✓	2 (AO2.5×2)	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous For C_2H_5–, ALLOW CH_3CH_2– For –CH=CH_2, ALLOW –C_2H_3 OR –$CHCH_2$ For bond into paper accept:  **ALLOW** two 3D structures with 2 groups swapped e.g.  **DO NOT ALLOW** a bond angle of 180° e.g.

					
		v	 ✓  ✓ **D** **E** 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	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 **Examiner's Comments** The majority of candidates were able to correctly define a structural isomer. This definition was well known by candidates with the majority of responses given the mark. Some candidates omitted the reference to structural formula. This question required candidates to link their knowledge of *cis* and *trans* isomers with branched hydrocarbons. Higher ability candidates were able to do this. The majority of candidates scored 1 mark for correctly drawing *cis* and *trans* isomers of an unbranched hydrocarbon. This question discriminated well. Candidates were required to identify the groups around a chiral carbon This question discriminated well. Candidates were required to identify the groups around a chiral carbon and then draw the two corresponding optical isomers. Incorrect responses frequently had incorrect connectivity around the chiral carbon, bond angles of 180° or 2D structures. Most candidates were able to correctly draw the structure of D and E. Many candidates did not explain their answers in terms of the number of different hydrogen and carbon

					environments or the presence/absence of a carbon-carbon double bond.
			Total	**10**	
12			**^{1}H NMR** δ = 1.1 ppm/doublet linked to 2 x C**H$_3$**✓ δ = 2.2 ppm/singlet linked to C**H$_3$**–C=O **OR** δ = 2.9 ppm/multiplet linked to C**H**$(CH_3)_2$ **OR H**C–C=O ✓ **Structure** Any structure with molecular formula $C_6H_{10}O_2$ and has 2 carbonyl groups ✓  ✓	4 (AO3.1×3) (AO3.2×1)	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **CHECK** spectra for annotations that may be worthy of credit **ALLOW** δ values ± 0.2 ppm, as a range or a value within the range **IGNORE H**C–C=O linked to δ = 2.2 ppm **IGNORE** additional chemical environments (taken from the data sheet) that align with the given chemical shifts **Examiner's Comments** This question proved difficult and although most candidates score some marks, only the very best responses secured all 4 marks. Candidates often did not link the doublet to two CH_3 groups and many only scored 1 mark for their suggested structure as the carbonyl groups were not side by side within the molecule.
			Total	**4**	
13		i	<table><tr><th>Proton environment</th><th>Splitting pattern</th><th></th></tr><tr><td>1</td><td>Triplet</td><td rowspan="2">Triplet **AND** quartet ✓</td></tr><tr><td>2</td><td>Quartet</td></tr><tr><td>3</td><td>Doublet</td><td rowspan="2">Doublet **AND** triplet ✓</td></tr><tr><td>4</td><td>Triplet</td></tr></table>	2 (2×AO1.2)	**For quartet,** **ALLOW Quad...**. e.g. **quad**ruplet, **quad**let, **quad**ret, etc For doublet, **ALLOW** duplet **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 **Examiner's Comments** This question tested candidates' ability to predict splitting patterns of an organic compound in a proton NMR spectrum. The 2 marks were given for the interacting protons in environments 1 and 2, and in environments 3

					and 4. Most candidates predicted the correct triplet/quartet splitting pattern for the common CH_3CH_2 group. The splitting pattern for the less common CH_2CHO was more difficult with many predicting at least one singlet. As with Question 1 (b) (ii), the second mark proved to be a very good discriminator.
		ii	**Environment 2:** (Protons) adjacent to (one) C=O ✓ **Environment 3:** (Protons) adjacent/between/surrounded by C=O / a ketone **AND** aldehyde **OR** C=O on both sides ✓ **2**	2 (2 ×AO3.1)	**ALLOW** HC-C=O **DO NOT ALLOW** H-C=O **DO NOT ALLOW** HC-O *Simply reading δ = 3.6 ppm from data sheet)* **IGNORE** 'next to 2 Os' **Examiner's Comments** This novel question required candidates to apply their knowledge and understanding of proton NMR spectroscopy to explain different chemical shifts. Most candidates used the *Data Sheet* in their answers, and most were then able to relate the chemical shift at δ = 2.5 ppm to an adjacent C=O group. Fewer candidates were then able to interpret the unexpected chemical shift at δ = 3.6 ppm to the presence of two adjacent C=O groups. Less successful responses often resorted to the *Data Sheet* a second time, suggesting the presence of an adjacent HC-O group, despite none being present in the structure. It was encouraging to see how many candidates were able to explain the two chemical shifts correctly, suggesting that most candidates are comfortable with this concept.
			Total	**4**	