

Mark scheme

Question	Answer/Indicative content	Marks	Guidance
1	<p><i>Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question.</i></p> <p>Level 3 (5-6 marks) Structure is C₆H₅CHCH₃CHO AND Analyses data from all 3 scientific points</p> <p><i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i></p> <p>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</p> <p><i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i></p> <p>Level 1 (1-2 marks) Attempts analysis from at least 2 of the scientific points</p> <p><i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i></p> <p>0 marks <i>No response or no response worthy of credit.</i></p>	6	<p>LOOK ON THE SPECTRA for labelled peaks and mark as SEEN</p> <p>Indicative scientific points:</p> <p><u>1. Empirical (and Molecular) Formulae</u></p> <ul style="list-style-type: none"> $\begin{aligned} \text{C:H:O} &= \frac{80.60}{12.0} : \frac{7.46}{1.0} : \frac{11.94}{16.0} \\ &= 6.72 : 7.46 : 0.746 \\ &= 9 : 10 : 1 \end{aligned}$ Empirical formula = C₉H₁₀O <p><u>2. Mass spectrum and IR</u></p> <p>Mass spectrum</p> <ul style="list-style-type: none"> uses $m/z = 134$ to give molecular formula: C₉H₁₀O Any possible fragments: <ul style="list-style-type: none"> $m/z = 105$ C₆H₅CHCH₃⁺ $m/z = 77$ C₆H₅⁺ $m/z = 29$ CHO⁺ <p>IR</p> <ul style="list-style-type: none"> C=O from ~1700 cm⁻¹ Likely to be aldehyde or ketone C=C (arenes) ~1500 cm⁻¹ <p>ALLOW Data Sheet ranges</p> <p><u>3. ¹H NMR</u></p> <ul style="list-style-type: none"> $\delta = 1.4$ ppm, doublet, 3H CH₃CH- $\delta = 3.8$ ppm, quintet, 1H next to 4 adjacent H $\delta = 7.3$ ppm, singlet, 5H C₆H₅⁻ $\delta = 9.0$ ppm, doublet, 1H -CHCHO

ALLOW approximate values for chemical shifts

Structure

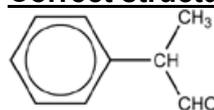
ALLOW any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous

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

Examiner's Comments

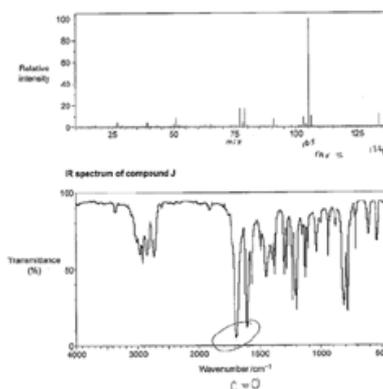
This question was well-attempted by most candidates, with the majority of candidates gaining full marks or gaining 4 marks for a top Level 2 response.

				<p>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.</p> <p>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.</p> <p>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 had fragments built up alongside their NMR analysis clearly building them using chemical shift, integration 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 at 3.8 ppm as being HC-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 CHO and the IR having C=C only without C=O as well.</p> <p>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: 'CH bonded to 'shifting groups' on either side, e.g. O-CH₂-C=O, may be shifted more than indicated above'.</p> <p>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</p>
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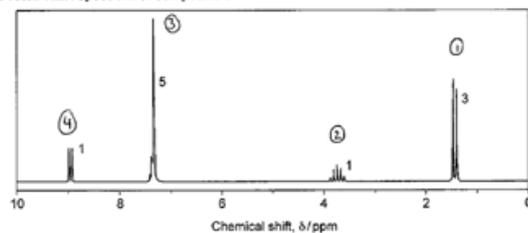
always ensure their final structure was clearly highlighted.

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



Proton NMR spectrum of compound J



The numbers by the peaks are the relative peak areas.

4 proton env

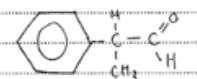
Determine the structure of compound J, showing all your reasoning. [6]

elemental analysis:

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

$$n(\text{H}) = \frac{7.46}{1} = 7.46 = 10 \quad \text{C}_9\text{H}_{10}\text{O} = 134$$

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

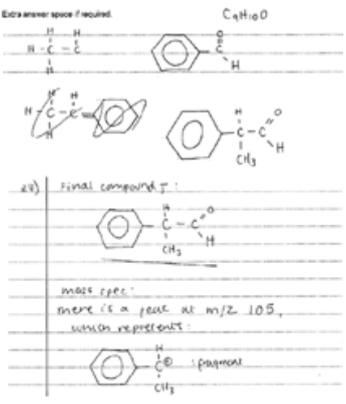


Infrared:

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

^1H NMR:

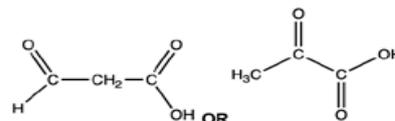
	ppm/δ	n of hydrogen	splitting	n of ppm on adjacent	
①	1.5	3	doublet	1	$\text{H}_3\text{C}-\text{CH}$
②	3.8	1	multiplet	4	$\text{HC}-\text{CH}_3$
③	7.3	5	doublet	0	C_6H_5
④	9.0	1	doublet	1	$-\text{C}(=\text{O})\text{H}$ (aldehyde)

				 <p>Extra answer space required.</p> <p>$C_9H_{10}O$</p> <p>Final compound:</p> <p>mass spec: there is a peak at m/z 105, which represents:</p> <p>fragment:</p>
				<p>Level 3, 6 marks</p> <p>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.</p>
			Total	6
2		A		<p>Examiner's Comments</p> <p>Most candidates gave the incorrect response D as their answer. Ultraviolet radiation does cause bonds in CFC molecules to break, and candidates may have been influenced by Question 8. However it is not a valid scientific reason for global warming. It suggests candidates may be confused about global warming verses the depletion of the ozone layer. This question was looking for candidates to link global warming to infrared active molecules i.e. C-H bond in methane.</p>

					<p>Just under a fifth of candidates gave the correct answer A.</p> <p> Misconception</p> <p>Many candidates believed there was a link between ultraviolet radiation and global warming. This is a topical issue so can be explored by looking at a range of resources including current news reports or exploring the United Nations resources.</p>
			Total	1	
3			D	1	<p><u>Examiner's Comments</u></p> <p>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.</p>
			Total	1	
4			B	1	<p><u>Examiner's Comments</u></p> <p>Some candidates correctly chose option B, with the other options being chosen randomly. From the importance placed on the causes of global warming, it was interesting to see that many incorrectly chose option A.</p> <p>Note also the points made in Question 6 about underlining the word 'not'.</p>
			Total	1	
5			C	1	<p><u>Examiner's Comments</u></p> <p>Most candidates first worked out the molecular mass of each fragment and</p>

				<p>annotated their scripts with this information, eliminating options A and C in the process. More successful responses than drew out the structure of the alcohol, to work out that only option C could have produced the fragment. This is evidence of good exam technique. Predictably, option B was the main distractor. This question discriminated well.</p>																					
			Total	1																					
6			<p>Level 3 (5-6 marks) A comprehensive description including most of the evidence to justify the correct structure of X.</p> <p><i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated</i></p> <p>Level 2 (3-4 marks) Explains two scientific points with few omissions OR some aspects from all three AND an attempt at a feasible structure with either a C=O OR COOH</p> <p><i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i></p> <p>Level 1 (1-2 marks) Determines the correct empirical/molecular formula OR Some aspects from two scientific points are given</p> <p><i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant</i></p> <p>0 marks - No response worthy of credit.</p>	6	<p>LOOK ON THE SPECTRA for labelled peaks. Indicative scientific points may include:</p> <p><u>1. Empirical formula</u></p> <table border="1"> <thead> <tr> <th>Element</th> <th>%mass</th> <th>Ar</th> <th>moles</th> <th>ratio</th> </tr> </thead> <tbody> <tr> <td>C</td> <td>40.91</td> <td>12</td> <td>3.41</td> <td>3</td> </tr> <tr> <td>H</td> <td>4.54</td> <td>1</td> <td>4.54</td> <td>4</td> </tr> <tr> <td>O</td> <td>54.55</td> <td>16</td> <td>3.41</td> <td>3</td> </tr> </tbody> </table> <p>Empirical formula = C₃H₄O₃ ALLOW Alternative method using M_r of 88 i.e. C = 88 x (40.91/100) x 12 = 3 etc.</p> <p><u>2. Spectra and Molecular formula</u></p> <p>Mass spectrum</p> <ul style="list-style-type: none"> molecular ion peak <i>m/z</i> or M_r = 88 molecular formula = C₃H₄O₃ <p>IR</p> <ul style="list-style-type: none"> peak at 2500 to 3500 cm⁻¹ is O-H peak at 1630 to 1820 cm⁻¹ is C=O <p><u>3. Functional groups and structure of X</u></p> <ul style="list-style-type: none"> X contains a carboxylic acid X doesn't decolourise Br₂ so no C=C bond Mass spectrum fragment peak(s) identified e.g. <ul style="list-style-type: none"> - <i>m/z</i> = 43 for CH₃CO⁺ - <i>m/z</i> = 29 CHO⁺ - <i>m/z</i> = 15 due to CH₃⁺ 	Element	%mass	Ar	moles	ratio	C	40.91	12	3.41	3	H	4.54	1	4.54	4	O	54.55	16	3.41	3
Element	%mass	Ar	moles	ratio																					
C	40.91	12	3.41	3																					
H	4.54	1	4.54	4																					
O	54.55	16	3.41	3																					

- **Structure of X**



Aspects of the communication statement might typically have been met when evidence is presented in a logical and clear order making good use of all the evidence given.

Some points which may be seen where communication is good include:

- Easy to follow layout on empirical formula calculation
- Empirical formula is same as molecular formula i.e. not given as $\text{CH}_{1.33}\text{O}$
- 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.
- No additional irrelevant/incorrect information given

Examiner's Comments

Over a third of candidates achieved Level 3, gaining 5 or 6 marks. A correct structure (either aldehyde or ketone) alone was not enough to award Level 3 and candidates were expected to give a comprehensive description of how the evidence helped them determine the structure.

The biggest challenge for many candidates was finding the correct empirical formula. The ratio worked out to 1:1.33:1 so many incorrectly rounded this to either 1:1:1 or 1:2:1, which meant they struggled to find a molecular formula that worked and added up to 88. Incorrect molecular formulas seen included $\text{C}_3\text{H}_3\text{O}_3$, which adds to 87 (often the extra H was just added to make it fit), or $\text{C}_4\text{H}_8\text{O}_2$, which does add to 88.

Most candidates could analyse the IR spectrum, identifying peaks corresponding to C=O or O-H. Candidates should identify bonds present before making conclusions

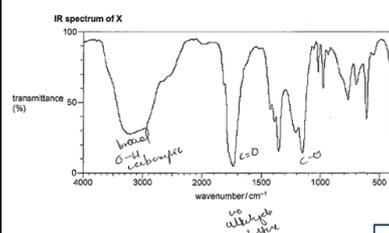
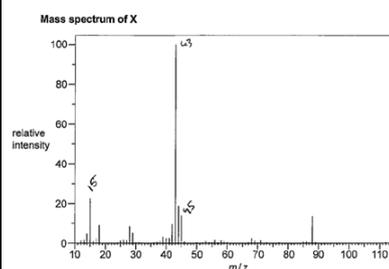
about the functional groups.

Many were able to use mass spectra to determine the M_r value from the M^+ peak. Some did go on to make use of other peaks, identifying fragments and confirming whether the structure was an aldehyde or ketone depending on analysis. For example, CHO^+ at $m/z = 29$ suggests an aldehyde, or conversely CH_3^+ at $m/z = 15$ suggests a ketone.

Candidates should always be encouraged to comment on all the data provided. This can be through good annotation of the spectra and notes added to the first page of the question. Many candidates didn't mention the evidence from the bromine test.

If candidates pieced together information to give a structure that is chemically feasible containing either a $\text{C}=\text{O}$ or COOH group then they could achieve Level 2. Without a structure they were limited to Level 1.

The most common incorrect structures seen included butanoic acid, 2-hydroxypropenoic acid or structures with $2 \times \text{C}=\text{O}$ and an alcohol OH .



Empirical formulae:

	C	H	O
mass	40.91	4.54	54.66
M_r	12	1	16
moles	3.41	4.54	3.41
ratio	1	1.3	1

$\text{CHO} = 29 \times 4 = \text{C}_4\text{H}_4\text{O}$

Molecular formulae

$$m/z = 88 \text{ (molecular mass)} = 88$$

$$\text{C}_4\text{H}_8\text{O}_2$$

mass spectroscopy = (fragment ions)

$$m/z 15 = \text{CH}_3^+$$

$$m/z 43 = \text{C}_3\text{H}_7^+$$

$$m/z 46 = \text{CH}_3\text{CH}_2\text{O}^+$$

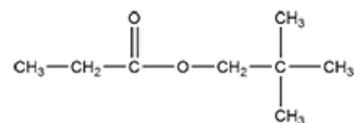
				<p>IR spectroscopy</p> <p>Extra answer space if required shows a broad peak of key absorption at 2500-3300 suggesting O-H of carboxylic acid shows an absorption at 1730-1820 for C=O of carboxylic acid, aldehyde etc. C-O (1000-1300) carboxylic acid.</p> <p>a) Compound X</p> <pre> H H H O H - C - C - C - C H H H O-H </pre> <p>butanoic acid</p>	
			Total	6	
7			C	1 (AO 2.5)	<p>Examiner's Comments</p> <p>Less than half the candidates interpreted which compound could have produced the IR spectrum. Many wrote the functional groups present alongside each option and all four options were seen in the responses. It was expected that the presence of a C=O absorption at 1700 cm⁻¹ would have led to A and B to be eliminated. Some thought that the peak at 3000 cm⁻¹ was for the carboxylic acid O-H which diverted some away from the correct option, C.</p>
			Total	1	
8			B	1 (AO 2.6)	<p>Examiner's Comments</p> <p>Candidates found this question a little easier and, as with previous organic questions, the best route to success was to draw out the structures of the organic isomers. For mass spectrum fragmentation, this ensures that the molecules can visually be split up into possible fragments. So well over half the candidates correctly identified the possible fragments and the correct option, B.</p>

		Total	1	
9		<p>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.</p> <p><i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i></p> <p>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.</p> <p><i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i></p> <p>Level 1 (1–2 marks) Attempts analysis from at least 2 of the scientific points.</p> <p><i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i></p> <p>0 mark No response or no response worthy of credit.</p>	<p>6 (AO1.2 × 2) (AO3.1 × 2) (AO3.2 × 2)</p>	<p>Mark spectra page as SEEN Indicative scientific points:</p> <p>1. Empirical Formulae</p> <ul style="list-style-type: none"> $\text{C} : \text{H} : \text{O} = \frac{66.63}{12.0} : \frac{11.18}{1.0} : \frac{22.19}{16.0}$ = 5.55 : 11.18 : 1.39 = 4 : 8 : 1 Empirical formula = $\text{C}_4\text{H}_8\text{O}$ <p>2. Molecular Formulae</p> <ul style="list-style-type: none"> uses $m/z = 144.0$ to determine molecular formula as $\text{C}_8\text{H}_{16}\text{O}_2$ <p>3. Functional group From IR,</p> <ul style="list-style-type: none"> → C=O from $\sim 1740 \text{ cm}^{-1}$ <p>IGNORE references to C–O peaks</p> <p>No reaction with 2,4-DNP</p> <ul style="list-style-type: none"> → no carbonyl/no ketone and aldehyde Likely to be an ester <p>4. ^1H NMR analysis</p> <ul style="list-style-type: none"> $\delta = 0.9 \text{ ppm}$, 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 $-\text{OCH}_2-$ <p>ALLOW approximate values for chemical shifts.</p> <p>Structure ALLOW any combination of skeletal OR structural OR displayed formula as long as <u>unambiguous</u></p> <p>Key features consistent with chemical shift data and relative peak areas</p> <ul style="list-style-type: none"> O-CH₂

- $C(CH_3)_3$
- $CH_3CH_2C=O$

Correct Structure

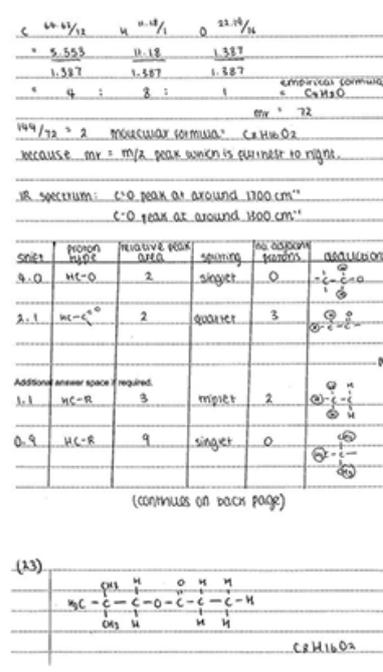
- $CH_3CH_2COOCH_2C(CH_3)_3$

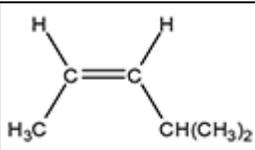
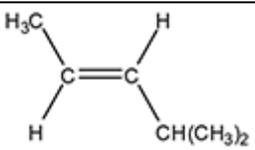
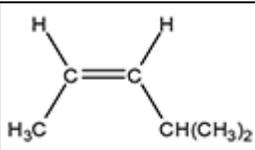
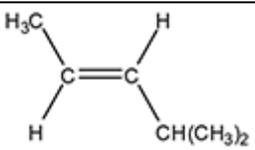
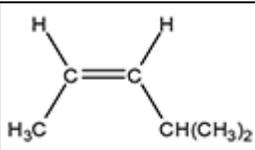
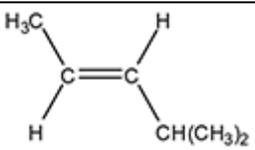


Examiner's Comments

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.

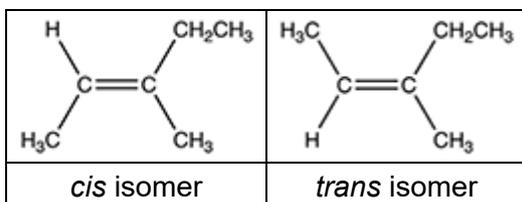
Good analysis of the NMR data was crucial for deducing the correct ester. Some candidates opted to annotate the proton NMR spectrum, some produced tables and others gave written details for each peak. It was vital that they were able to interpret all information for each peak i.e. number of proton environments, 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

				<p>$(\text{CH}_3)_3\text{COCH}_2\text{COCH}_2\text{CH}_3$ or not checking it matched the molecular formula $\text{CH}_3\text{CH}_2\text{COOC}(\text{CH}_3)_3$ so only achieved Level 1.</p> <p>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.</p> <p>Exemplar 3</p>  <p>The handwritten response shows a student's analysis of NMR data. At the top, they list chemical shifts: $\delta = 4.4/12$, $\delta = 1.8/1$, and $\delta = 2.1/4$. Below this is a table with columns for chemical shift, integration, and assignment. The table shows three peaks: a singlet at $\delta = 4.0$ (3H, O=C-O), a quartet at $\delta = 2.1$ (2H, H-C-O), and a singlet at $\delta = 0.9$ (9H, H-C-R). The student also notes IR peaks at 1700 cm^{-1} (C=O) and 1300 cm^{-1} (C-O). At the bottom, they draw the chemical structure of 2,2,4,4-tetramethylpentane-3-one, $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{O})\text{CH}_2\text{C}(\text{CH}_3)_3$, and label it as $\text{C}_8\text{H}_{16}\text{O}_2$.</p>
		Total	6	
10		B	1 (AO2.1)	
		Total	1	
11		C	1 (AO2.1)	<p>Examiner's Comments</p> <p>Many gained credit here but as A was the most common incorrect response it demonstrates the need to make sure</p>

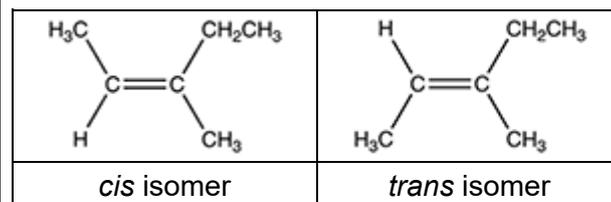
					candidates can recognise the difference between an alcoholic O-H and carboxylic acid O-H in IR.				
			Total	1					
12			B	1 (AO2.5)	Examiner's Comments Most candidates correctly identified C as the compound after labelling the peaks in the spectrum.				
			Total	1					
13		i	<p>Same molecular formula AND Different structural formulae ✓</p> <p>OR</p> <p>Both have the molecular formula C₆H₁₂ AND Different structural formulae ✓</p>	1 (AO1.1)	<p>Same formula is not sufficient</p> <p>(no reference to molecular) Different arrangement of atoms is not sufficient</p> <p>(no reference to structure/structural)</p> <p>For 'structural formulae', ALLOW structure/displayed/skeletal formulae/functional groups</p> <p>DO NOT ALLOW any reference to spatial/space</p>				
		ii	<p>Same structural formula AND Different arrangement (of atoms) in space OR different spatial arrangement (of atoms) ✓</p>	1 (AO1.1)	<p>ALLOW structure/displayed/skeletal formula</p> <p>DO NOT ALLOW same empirical formula OR same general formula</p> <p>IGNORE same molecular formula</p> <p>Reference to <i>E/Z</i> isomerism or optical isomerism is not sufficient</p>				
		iii	<p>Correct identification of <i>cis</i> AND <i>trans</i> isomers of 4-methylpent-2-ene ✓✓</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <tr> <td style="text-align: center;">  </td> <td style="text-align: center;">  </td> </tr> <tr> <td style="text-align: center;"><i>cis</i> isomer</td> <td style="text-align: center;"><i>trans</i> isomer</td> </tr> </table>			<i>cis</i> isomer	<i>trans</i> isomer	2 (AO1.2) (AO2.5)	<p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>C₃H₇ is not sufficient (could be unbranched)</p> <p>ALLOW one mark if <i>cis</i> AND <i>trans</i> isomers of 4-methylpent-2-ene are in the wrong boxes</p>
									
<i>cis</i> isomer	<i>trans</i> isomer								

OR

Identification of 3-methylpent-2-ene as *cis* AND *trans* isomers ✓✓

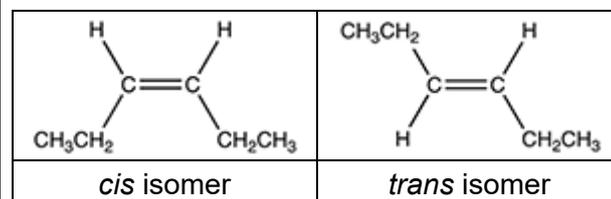


ALLOW the isomers of 3-methylpent-2-ene in either box

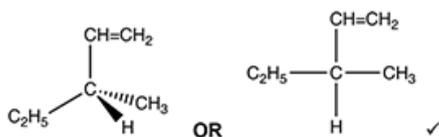


Ambiguity with cis/trans identification system

ALLOW one mark for correct identification of *cis*
AND *trans* isomers of unbranched C₆H₁₂
e.g.

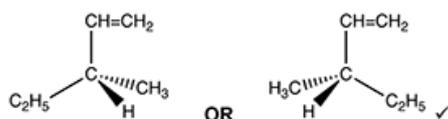


Correct groups attached to chiral carbon of compound C seen **once** e.g.



iv

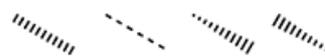
Two **3D structures** of compound C that are mirror images with correct connectivity in both



ALLOW any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous

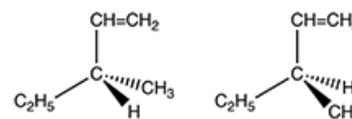
For C₂H₅–, ALLOW CH₃CH₂–
For –CH=CH₂, ALLOW –C₂H₃ OR –CHCH₂

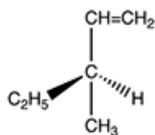
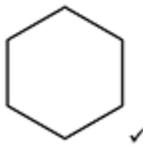
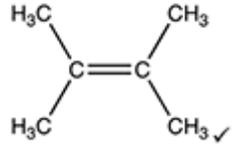
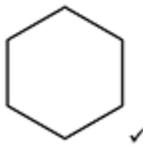
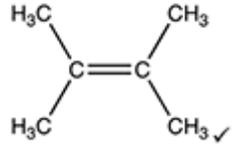
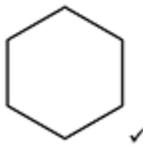
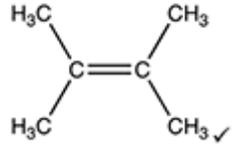
For bond into paper accept:



2
(AO2.5×2
)

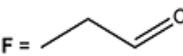
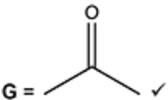
ALLOW two 3D structures with 2 groups swapped
e.g.



				<p>DO NOT ALLOW a bond angle of 180° e.g.</p> 				
			<table border="1" data-bbox="223 795 742 996"> <tr> <td></td> <td></td> </tr> <tr> <td style="text-align: center;">D</td> <td style="text-align: center;">E</td> </tr> </table> <p>Two of the following for D ✓</p> <ul style="list-style-type: none"> • 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 <p>Two of the following for E ✓</p> <ul style="list-style-type: none"> • All H are equivalent/ in the same chemical environment/ the same type • 2 C environments • C=C present 			D	E	<p>ALLOW 1 mark for structures if shown in wrong boxes.</p> <p>CHECK table 16.1 for annotations that may be worthy of credit</p> <p>Examiner's Comments</p> <p>The majority of candidates were able to correctly define a structural isomer.</p> <p>This definition was well known by candidates with the majority of responses given the mark. Some candidates omitted the reference to structural formula.</p> <p>This question required candidates to link their knowledge of <i>cis</i> and <i>trans</i> isomers with branched hydrocarbons. Higher ability candidates were able to do this. The majority of candidates scored 1 mark for correctly drawing <i>cis</i> and <i>trans</i> isomers of an unbranched hydrocarbon.</p> <p>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.</p> <p>Most candidates were able to correctly draw</p>
								
D	E							

v

4
(AO2.5×2)
(AO2.2×2)

					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	
14			<p>Initial ratios $C, \frac{62.07}{12.0} : H, \frac{10.34}{1.0} : O, \frac{27.59}{16.0}$</p> <p>OR</p> <p>C, 5.1725 : H, 10.34 : O, 1.724</p> <p>OR</p> <p>C, 3 : H, 6 : O, 1 ✓</p> <p>(Molecular formula =) C₃H₆O</p> <p>AND Evidence of 58 in working or from labelled peak in one of the spectra ✓</p> <p>For F evidence for fragment ion m/z=29 linked to CH₃CH₂(⁺) OR CHO(⁺) ✓</p> <p>F = </p> <p>AND</p> <p>G = </p>	<p>4 (AO1.2) (AO2.5) (AO3.2) (AO3.2)</p>	<p>CHECK spectra for annotations that may be worthy of credit</p> <p>Mark can be awarded from a correct molecular formula</p> <p>IGNORE m/z=15 (as this is not unique) IGNORE m/z=43</p> <p>IGNORE incorrect fragments IGNORE charges on fragment ions</p> <p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>Examiner's Comments</p> <p>Most candidates were able to calculate the initial ratios and then use this to calculate the molecular formula, linking to the m/z peak at 58. The most common error seen was for the structures of F and G to be in the incorrect boxes, suggesting that candidates have not interpreted the fragment ions to work out F was the aldehyde.</p>
			Total	4	
15			B	<p>1 (AO1.1)</p>	<p>Examiner's Comments</p> <p>Candidates found this multiple choice</p>

				question challenging. While some identified B as the correct answer, many candidates selected C.																				
			Total	1																				
16		A	1(AO2.5)	<p><u>Examiner's Comments</u></p> <p>Candidates found this question hard with many selecting C or D instead of the correct option, B. Candidates appeared to have assigned the C–H absorption at 3000 cm^{-1} to an O–H group (from an alcohol or carboxylic acid). Candidates should appreciate that this C–H absorption will be present in any organic compound possessing a C–H group (that is, nearly all organic compounds).</p>																				
			Total	1																				
17		<p>Level 3 (5-6 marks) A comprehensive description including most of the evidence to justify the correct structure of A (accept <i>cis</i> or <i>trans</i>).</p> <p><i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i></p> <p>Level 2 (3-4 marks) Explains two scientific points thoroughly with few omissions. AND an attempt at a feasible structure with either a C=C OR COOH</p> <p><i>There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.</i></p> <p>Level 1 (1-2 marks) The correct empirical formula AND a simple description based on at least one of the main scientific points. OR Some aspects from two scientific points are given</p> <p><i>There is an attempt at a logical structure with a line of reasoning. The</i></p>	<p>6 (AO 3.1 × 3) (AO 3.2 × 3)</p>	<p>LOOK AT THE SPECTRA for labelled peaks Indicative scientific points may include:</p> <p><u>Empirical formula</u> • empirical formula = C₂H₃O</p> <table border="1"> <thead> <tr> <th>element</th> <th>%mass</th> <th>A_r</th> <th>moles</th> <th>ratio</th> </tr> </thead> <tbody> <tr> <td>C</td> <td>55.8</td> <td>12</td> <td>4.65</td> <td>2</td> </tr> <tr> <td>H</td> <td>7.0</td> <td>1</td> <td>7.0</td> <td>3</td> </tr> <tr> <td>O</td> <td>37.2</td> <td>16</td> <td>2.325</td> <td>1</td> </tr> </tbody> </table> <p><u>Spectra and molecular formula</u> Mass spectrum</p> <ul style="list-style-type: none"> • (molecular ion peak $m/z = 86$) • molar mass = 86 g mol^{-1} • molecular formula = C₄H₆O₂ <p>Infrared absorption;</p> <ul style="list-style-type: none"> • broad peak at $2500\text{--}3300\text{ cm}^{-1}$, due to O–H in carboxylic acid, • peak at $1630\text{--}1820\text{ cm}^{-1}$ due to C=O (peak at $1620\text{--}1680\text{ cm}^{-1}$ due to C=C) • <u>Functional groups, structure and stereochemistry</u> <ul style="list-style-type: none"> • alkene / C=C • carboxylic acid / –COOH 	element	%mass	A _r	moles	ratio	C	55.8	12	4.65	2	H	7.0	1	7.0	3	O	37.2	16	2.325	1
element	%mass	A _r	moles	ratio																				
C	55.8	12	4.65	2																				
H	7.0	1	7.0	3																				
O	37.2	16	2.325	1																				

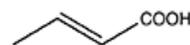
information is in the most part relevant.

0 marks No response or no response worthy of credit.

- mass spectrum; peak at 41 due to loss of COOH
- Correct structural formula:
 $\text{CH}_3\text{CH}=\text{CHCOOH}$

i.e. *cis* **OR** *trans*

- *trans* isomer indicates C=C bond with 2 different groups attached to both double bonded carbons
- *trans*: common groups on opposite sides of double bond
- Correct structure:



NOTE: Correct *trans* assignment with justification would be an example of a well-developed line of reasoning that is substantiated.

Examiner's Comments

About a third of candidates were given Level 3 for this question. The key to answering this style of question well is to make sure all the information provided is used and to avoid contradictory statements, e.g. "structure contains carboxylic acid from IR" but then not present in final structure drawn, or a structure that doesn't match the molecular formula given. A significant number of candidates did not include C=C despite being told in the question that it was "unsaturated and is a *trans* stereoisomer", plus the C=C bond is shown in the IR and molecular formula needed unsaturation. The M+1 peak did confuse some candidates who then tried to add an extra H to final structure. It is very important that any structure given is feasible in terms of bonding; many candidates gave structures with C with 5 bonds (with both C=C and C=O attached), limiting them to achieving only L1. Some candidates gave a *cis* structure rather than *trans*.

Other candidates ignored the O-H peak (from the carboxylic acid) in the IR spectrum, attributing this to a C-H bond as it was not as smooth or as prominent as they may have

seen in other spectra. Some listed the bonds observed in the IR without linking to their position – this can easily be done by annotating the spectra.

Many candidates had messy answers with lots of rough working which was then not crossed out – this made their answer very confusing. Note that no marks were given for just the empirical formula calculation and some attempted to produce a structure from the empirical formula without determining the M_r from the M^+ peak in mass spectrum.

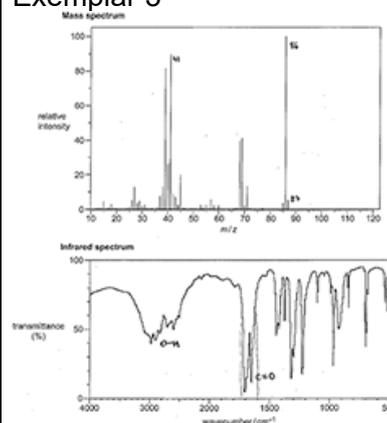


OCR support

We have put together a range of online resources to support teaching of organic chemistry:

<https://www.ocr.org.uk/qualifications/as-a-level-gce-chemistry-a-h032-h432-from-2015/deliveryguide/module-cam04-module-4-core-organic-chemistry/delivery-guide-cadg012-organicchemistry-as>

Exemplar 3



C	H	O	Empirical formula: C ₅ H ₆ O
55.2	7.6	37.2	86
11	1	16	43
2.85	2.0	2.365	
1.355	1.355	1.355	Molecular formula: C ₁₀ H ₁₂ O ₂
1	1	1	



Compound A has an empirical formula of C₅H₆O but the relative molecular mass is 86 so the molecular formula is C₁₀H₁₂O₂. It is a trans isomer so it has a C=C double bond. Compound A has an O-H peak between 2500-3500 and a C=O peak between 1650-1750. Therefore it is a carboxylic acid. The most stable isomer of compound A is ~~C₁₀H₁₂O₂~~ C₁₀H₁₂O₂ which has a m/z of 86. Therefore compound A is:



This is an example of a good response which achieved L3 6 marks. Empirical and molecular

					formula are determined. Spectra have been annotated to aid their interpretation, but they have also included the key IR peaks as well as a MS fragment in their response. The correct structure for A is clearly drawn out. The response is clear and concise, with all information presented being relevant.
			Total	6	