

**GCE**

**Chemistry A**

**H432/02:** Synthesis and analytical techniques

Advanced GCE

**Mark Scheme for November 2020**

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




This mark scheme is published as an aid to teachers and students, to indicate the requirements of the examination. It shows the basis on which marks were awarded by examiners. It does not indicate the details of the discussions which took place at an examiners' meeting before marking commenced.

All examiners are instructed that alternative correct answers and unexpected approaches in candidates' scripts must be given marks that fairly reflect the relevant knowledge and skills demonstrated.

Mark schemes should be read in conjunction with the published question papers and the report on the examination.

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## 1. Annotations available in RM Assessor

Annotation	Meaning
	Correct response
	Incorrect response
	Omission mark
	Benefit of doubt given
	Contradiction
	Rounding error
	Error in number of significant figures
	Error carried forward
	Level 1
	Level 2
	Level 3
	Benefit of doubt not given
	Noted but no credit given
	Ignore

2. Abbreviations, annotations and conventions used in the detailed Mark Scheme (to include abbreviations and subject-specific conventions).

<b>Annotation</b>	<b>Meaning</b>
<b>DO NOT ALLOW</b>	Answers which are not worthy of credit
<b>IGNORE</b>	Statements which are irrelevant
<b>ALLOW</b>	Answers that can be accepted
( )	Words which are not essential to gain credit
—	Underlined words must be present in answer to score a mark
<b>ECF</b>	Error carried forward
<b>AW</b>	Alternative wording
<b>ORA</b>	Or reverse argument

## 1. Subject-specific Marking Instructions

### INTRODUCTION

Your first task as an Examiner is to become thoroughly familiar with the material on which the examination depends. This material includes:

- the specification, especially the assessment objectives
- the question paper
- the mark scheme.

You should ensure that you have copies of these materials.

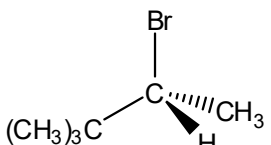
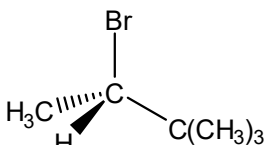
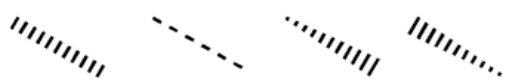
You should ensure also that you are familiar with the administrative procedures related to the marking process. These are set out in the OCR booklet **Instructions for Examiners**. If you are examining for the first time, please read carefully **Appendix 5 Introduction to Script Marking: Notes for New Examiners**.

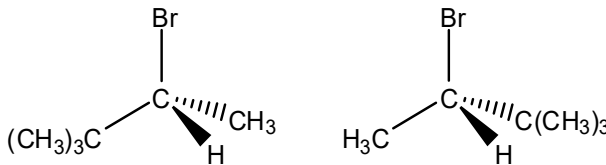
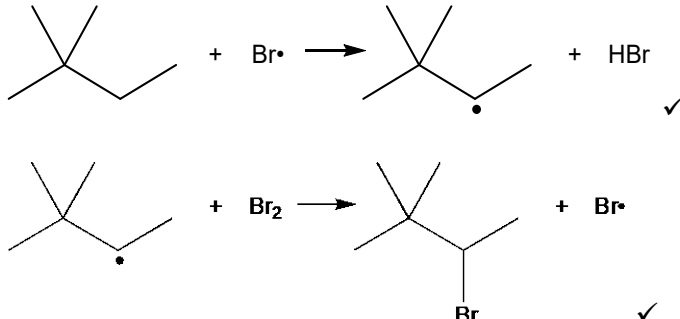
Please ask for help or guidance whenever you need it. Your first point of contact is your Team Leader.

## SECTION A

Question	Answer	Marks	AO element	Guidance
1	A	1	1.2	
2	B	1	1.1	
3	A	1	1.1	
4	C	1	2.3	
5	D	1	1.2	
6	D	1	2.1	
7	A	1	1.1	
8	C	1	2.2	
9	D	1	1.2	
10	C	1	2.5	ALLOW 5
11	A	1	2.6	
12	A	1	2.2	
13	A	1	1.1	
14	B	1	2.3	
15	C	1	1.2	

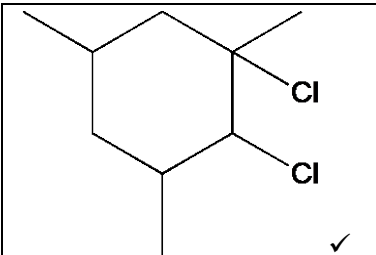
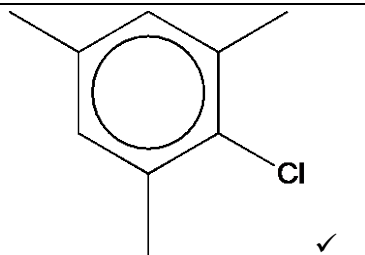
## SECTION B

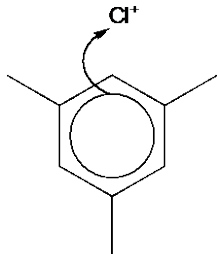
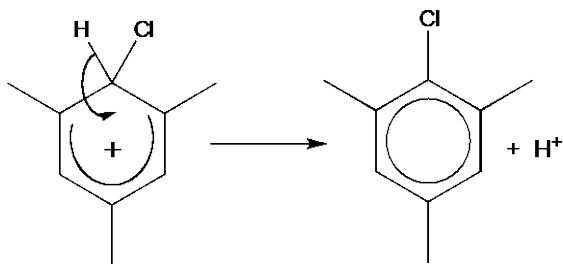
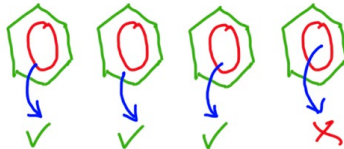
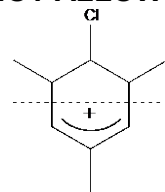
Question			Answer	Marks	AO element	Guidance
16	(a)	(i)	2-bromo-3,3-dimethylbutane ✓	1	1.2	<p><b>IGNORE</b> lack of hyphens or addition of commas</p> <p><b>ALLOW</b> 3,3-dimethyl-2-bromobutane</p> <p><b>DO NOT ALLOW</b>            2-bromo-3-dimethylbutane            methy for methyl            methly for methyl            brom for bromo</p>
	(b)	(i)	<p><b>Stereoisomers</b>            Same structural formula  <b>AND</b>            Different arrangement (of atoms) in space  <b>OR</b> different spatial arrangement (of atoms)  <b>AND</b>  <b>Type: Optical</b> ✓</p>	1	1.2	<p><b>ALLOW</b> structure/displayed/skeletal formula</p> <p><b>DO NOT ALLOW</b> same empirical formula  <b>OR</b> same general formula</p> <p><b>IGNORE</b> same molecular formula  <b>IGNORE</b> references to chiral molecules/compounds</p>
		(ii)	<p>One 3D structure with correct groups attached to the chiral C ✓</p> <p>Two 3D structures of <math>(\text{CH}_3)_3\text{CCHBrCH}_3</math> that are mirror images <b>AND</b> correct connectivity in both ✓</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  </div> <div style="text-align: center;">  </div> </div>	2	<p><b>2.5</b></p> <p><b>1.2</b></p>	<p><b>ALLOW</b> small slip in one of the groups OR use of <math>\text{C}_4\text{H}_9</math>            3D structures must have four central bonds with <b>at least two wedges</b>.</p> <p>For bond into paper accept:</p> <div style="text-align: center;">  </div> <p><b>ALLOW</b> two 3D structures with 2 groups swapped e.g.</p>

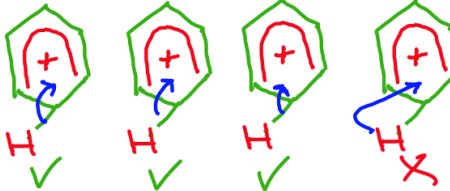
Question			Answer	Marks	AO element	Guidance
						
(c)		<div><div><b>Initiation</b> <math>\text{Br}_2 \rightarrow 2\text{Br}\cdot</math> ✓</div><div><b>Propagation</b> </div></div>	3	1.2  		

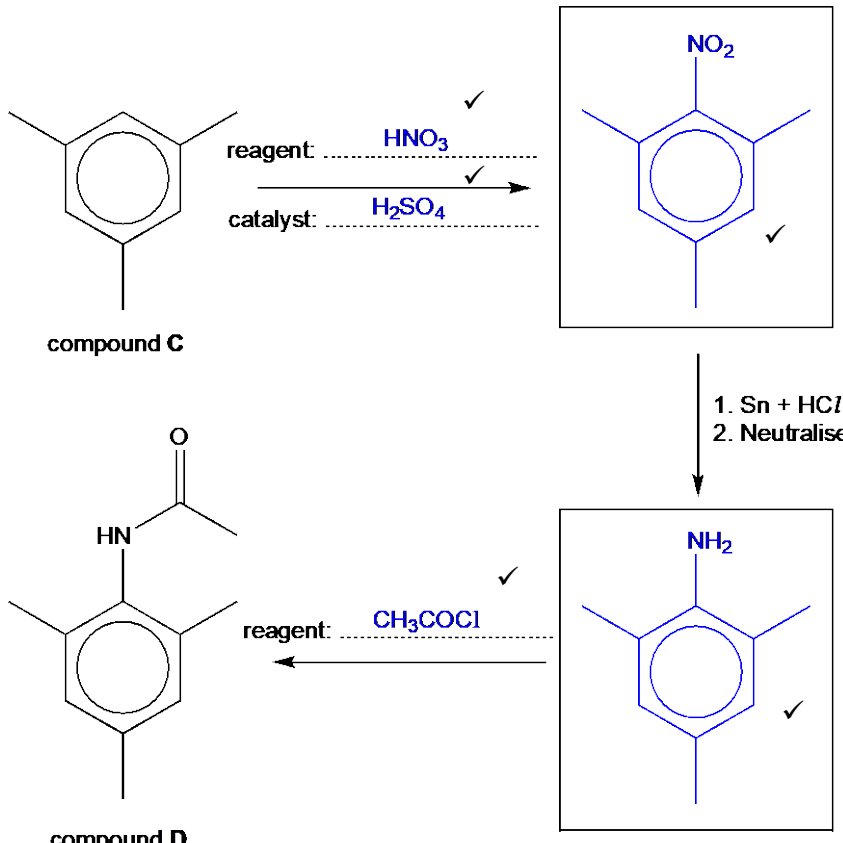


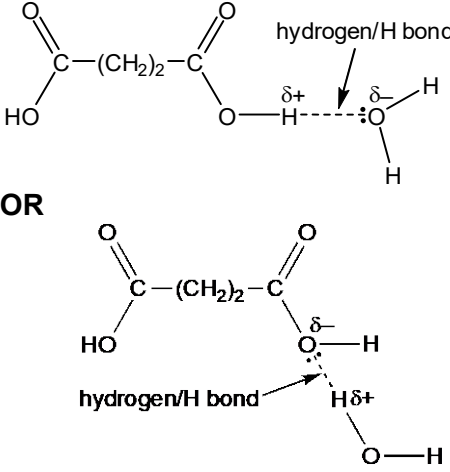
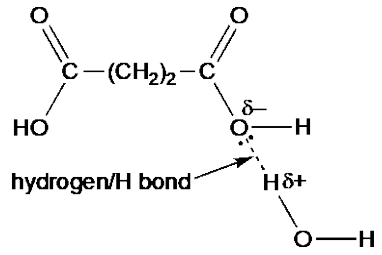
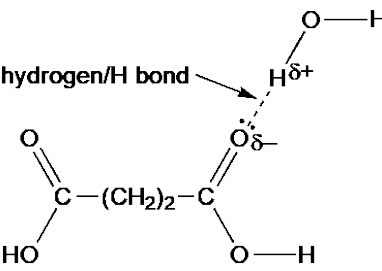
Question			Answer	Marks	AO element	Guidance
	(d)		<p>further substitution/s  <b>OR</b>  produces different termination products  <b>OR</b>  More than one termination step  <b>OR</b>  Mixture of products are formed ✓</p> <p>substitution at different positions along chain ✓</p>	2	1.1×2	<p><b>ALLOW</b> dibromo/multibromo compounds formed  <b>OR</b> an example of a further substitution product  <b>OR</b> an example of a different termination product  <b>ALLOW</b> more than one hydrogen (atom) can be replaced  <b>ALLOW</b> radicals react with each other to form other products  <b>IGNORE</b> references to separation of products  <b>IGNORE</b> references to atom economy or yield</p> <p><b>ALLOW</b> a hydrogen (atom) on a different carbon (atom) can be replaced</p>

Question			Answer	Marks	AO element	Guidance
17	(a)	(i)	<div>   Organic product with <b>B</b> </div> <div>   Organic product with <b>C</b> </div>	2	2.5×2	
		(ii)	<p><b>Reactivity of B</b>  in B electrons are localised  OR  in B <math>\pi</math>-bond is localised ✓</p> <p><b>Reactivity of C</b>  in C electrons are delocalised  OR  In C <math>\pi</math>-system / ring is delocalised</p> <p>In <b>B</b>, electron density is higher  <b>AND</b>  B is more susceptible to electrophilic attack  <b>OR</b>  B attracts/accepts the electrophile/<math>\text{Cl}_2</math> more  <b>OR</b>  B polarises the electrophile/<math>\text{Cl}_2</math> more ✓  <b>ORA</b></p>	3	1.1×3	<p><b>ALLOW</b> labelled diagram to show delocalised system</p> <p><b>IGNORE</b> charge density  <b>IGNORE</b> electronegativity</p> <p><b>IGNORE</b> B is more reactive/reacts more readily (no reference to electrophile)</p> <p><b>IGNORE</b> references to electron density spread around the <math>\pi</math>-ring</p> <p><b>ALLOW</b> chlorine</p>

Question	Answer	Marks	AO element	Guidance
(iii)	<p><b>Generation of electrophile</b></p> $\text{AlCl}_3 + \text{Cl}_2 \rightarrow \text{AlCl}_4^- + \text{Cl}^+ \checkmark$ <p><b>Attack of <math>\text{Cl}^+</math></b></p>  <p>Curly arrow from <math>\pi</math>-bond to <math>\text{Cl}^+</math> <math>\checkmark</math></p> <hr/> <p><b>Intermediate and organic product</b></p>  <p>Correct intermediate <math>\checkmark</math></p> <p>Curly arrow from C-H bond to reform <math>\pi</math>-ring <math>\checkmark</math></p> <hr/> <p><b>Regeneration of catalyst</b></p> $\text{H}^+ + \text{AlCl}_4^- \rightarrow \text{AlCl}_3 + \text{HCl} \checkmark$	5	<p>1.2</p> <p>1.2</p> <p>1.2</p> <p>2.5</p> <p>1.2</p> <p>1.2</p>	<p><b>ANNOTATE ANSWER WITH TICKS AND CROSSES</b></p> <p><b>ALLOW</b> <math>\text{FeCl}_3 + \text{Cl}_2 \rightarrow \text{FeCl}_4^- + \text{Cl}^+</math></p> <p><b>ALLOW</b> use of Fe</p> <p><b>NOTE:</b> curly arrows can be straight, snake-like, etc. ..... but <b>NOT</b> double-headed or half-headed arrows</p> <p><b>1st curly arrow</b> must</p> <ul style="list-style-type: none"> <li>start from, <b>OR</b> close to, <b>circle of benzene ring</b></li> </ul>  <p><b>DO NOT ALLOW</b> following intermediate:</p>  <p><math>\pi</math>-ring must cover 4 of the 6 sides of the benzene ring <b>AND</b> correct orientation, <i>i.e.</i> gap towards C-Cl</p> <p><b>ALLOW</b> + sign anywhere inside the 'hexagon' of the intermediate.</p>

Question			Answer	Marks	AO element	Guidance						
						<p><b>IGNORE</b> partial charges on the chlorine in the intermediate</p> <p><b>DO NOT ALLOW</b> mark for intermediate if any CH<sub>3</sub> is missing</p> <p><b>Curly arrow</b> must start from, <b>OR</b> be traced back to, <b>any part of</b> C-H bond and go inside the 'hexagon'</p>  <p><b>ALLOW</b> use of AlCl<sub>4</sub><sup>-</sup> in the mechanism</p> <p><b>ALLOW</b> ECF for regeneration of an incorrect metal chloride catalyst e.g. AgCl<sub>3</sub></p>						
	(b)		<p>3C<sub>3</sub>H<sub>6</sub>O → C<sub>9</sub>H<sub>12</sub> + 3H<sub>2</sub>O</p> <p>molecular formulae of C<sub>3</sub>H<sub>6</sub>O <b>AND</b> C<sub>9</sub>H<sub>12</sub> ✓</p> <p>H<sub>2</sub>O as by-product ✓</p> <p>correct balanced equation ✓</p>	3		<p>2.6</p> <p>2.5</p> <p>2.6</p>						
	(c)	(i)	<table><tr><td></td><td>Compound C</td><td>Compound D</td></tr><tr><td>Number of peaks</td><td>3 ✓</td><td>8 ✓</td></tr></table>		Compound C	Compound D	Number of peaks	3 ✓	8 ✓	2	3.2	
	Compound C	Compound D										
Number of peaks	3 ✓	8 ✓										

Question	Answer	Marks	AO element	Guidance
(ii)	 <p>compound C</p> <p>reagent: <math>\text{HNO}_3</math></p> <p>catalyst: <math>\text{H}_2\text{SO}_4</math></p> <p>1. Sn + HCl 2. Neutralise</p> <p>reagent: <math>\text{CH}_3\text{COCl}</math></p> <p>compound D</p>	5	3.2×5	<p><b>ALLOW</b> any combination of skeletal <b>OR</b> structural <b>OR</b> displayed formula as long as unambiguous</p> <p><b>IGNORE</b> names for organic intermediates (question asks for structures)</p> <p><b>ALLOW</b> names of reagents and catalyst</p> <p>Around top arrow, <b>ALLOW</b> 1 of 2 marks if <math>\text{HNO}_3</math> and <math>\text{H}_2\text{SO}_4</math> swapped. i.e.</p> <p>reagent: <math>\text{H}_2\text{SO}_4</math></p> <p>catalyst: <math>\text{HNO}_3</math></p> <p><b>IGNORE</b> references to concentration</p> <p><b>ALLOW</b> <math>(\text{CH}_3\text{CO})_2\text{O}</math> for left arrow</p> <p><b>IGNORE</b> <math>\text{CH}_3\text{COOH}</math> <b>IGNORE</b> acyl chloride</p> <p><b>DO NOT ALLOW</b> <math>\text{AlCl}_3/\text{FeCl}_3/\text{Fe4}</math></p>

Question	Answer	Marks	AO element	Guidance
18 (a) (i)	<p><b>Reagents</b>  <math>\text{K}_2\text{Cr}_2\text{O}_7</math> <b>AND</b> acid  <b>AND</b> reflux ✓</p> <p><b>Equation</b>  <math>\text{HO}(\text{CH}_2)_4\text{OH} + 4[\text{O}] \rightarrow \text{HOOC}(\text{CH}_2)_2\text{COOH} + 2\text{H}_2\text{O}</math></p> <p><math>[\text{O}]</math> <b>AND</b> <math>\text{H}_2\text{O}</math> ✓</p> <p>Correctly balanced equation ✓</p>	3	1.1      2.5  2.6	<p><b>ALLOW</b> <math>\text{Na}_2\text{Cr}_2\text{O}_7</math> <b>OR</b> <math>\text{Cr}_2\text{O}_7^{2-}</math>  <b>ALLOW</b> <math>\text{H}_2\text{SO}_4</math> <b>OR</b> <math>\text{HCl}</math> <b>OR</b> <math>\text{H}^+</math>  <b>ALLOW</b> words. e.g. 'acidified dichromate'  <b>ALLOW</b> a small slip in formula for dichromate e.g <math>\text{KCr}_2\text{O}_7</math>,</p>
	<p>(ii)</p>  <p>OR</p>  <p>Diagram showing correct dipole charges on each end of one hydrogen bond between a water molecule and a diacid ✓</p> <p>Hydrogen bond between one lone pair on O atom in one of the molecules and the H atom of another  <b>AND</b>  Hydrogen bonding stated or labelled on diagram</p>	2	2.1×2	<p><b>ALLOW</b> any combination of skeletal <b>OR</b> structural <b>OR</b> displayed formula as long as unambiguous</p> <p><b>DO NOT ALLOW</b> <math>\delta+</math> on H atoms of <math>\text{CH}_2</math> group</p> <p><b>ALLOW</b> H-bond for hydrogen bond</p> <p><b>ALLOW</b> H bond between <math>\text{C}=\text{O}</math> and <math>\text{H}_2\text{O}</math>, i.e.</p>  <p><b>IF</b> diagram is not labelled, <b>ALLOW</b> hydrogen bond/H bond from text</p>

Question		Answer	Marks	AO element	Guidance
(b)	(i)	$\text{-----}\overset{\text{O}}{\parallel}\text{C}-(\text{CH}_2)_2-\overset{\text{O}}{\parallel}\text{C}-\text{O}-(\text{CH}_2)_4-\text{O} \text{-----}$ <p>Ester link (must be displayed) ✓</p> <p>Rest of structure ✓</p>	2	1.2 2.5	<p><b>ALLOW</b> the 'O' or C=O at either end, e.g.</p> $\text{---O---}\overset{\text{O}}{\parallel}\text{C}-(\text{CH}_2)_2-\overset{\text{O}}{\parallel}\text{C}-\text{O}-(\text{CH}_2)_4\text{---}$ $\text{---}(\text{CH}_2)_2-\overset{\text{O}}{\parallel}\text{C}-\text{O}-(\text{CH}_2)_4-\text{O}-\overset{\text{O}}{\parallel}\text{C} \text{---}$ <p><b>IGNORE</b> brackets</p> <p><b>IGNORE</b> <math>n</math></p> <p>End bonds' <b>MUST</b> be shown (solid or dotted)</p> <p><b>DO NOT ALLOW</b> more than one repeat unit</p>
	(ii)	<p>the ester/ ester bond/ ester group /polyester can be broken down ✓</p> <p><b>OR</b></p> <p>It can be hydrolysed ✓</p>	1	3.2	<p><b>IGNORE</b> references to photodegradable</p> <p>'Bond breaks' is not sufficient – no reference to ester bond</p>
	(iii)	$\begin{array}{c} \text{O} & & \text{O} \\ \parallel & & \parallel \\ \text{HO}-\text{C}-(\text{CH}_2)_2-\text{C}-\text{OH} \end{array} + 2 \text{SOCl}_2 \longrightarrow \begin{array}{c} \text{O} & & \text{O} \\ \parallel & & \parallel \\ \text{Cl}-\text{C}-(\text{CH}_2)_2-\text{C}-\text{Cl} \end{array} + 2 \text{SO}_2 + 2 \text{HCl}$ <p>SOCl<sub>2</sub> in equation ✓</p> <p>Structure of diacyl dichloride ✓</p> <p>Complete balanced equation ✓</p>	3	1.1 1.2 2.6	<p><b>ALLOW</b> alternative approach using PCl<sub>5</sub> or PCl<sub>3</sub></p>

[illegible]

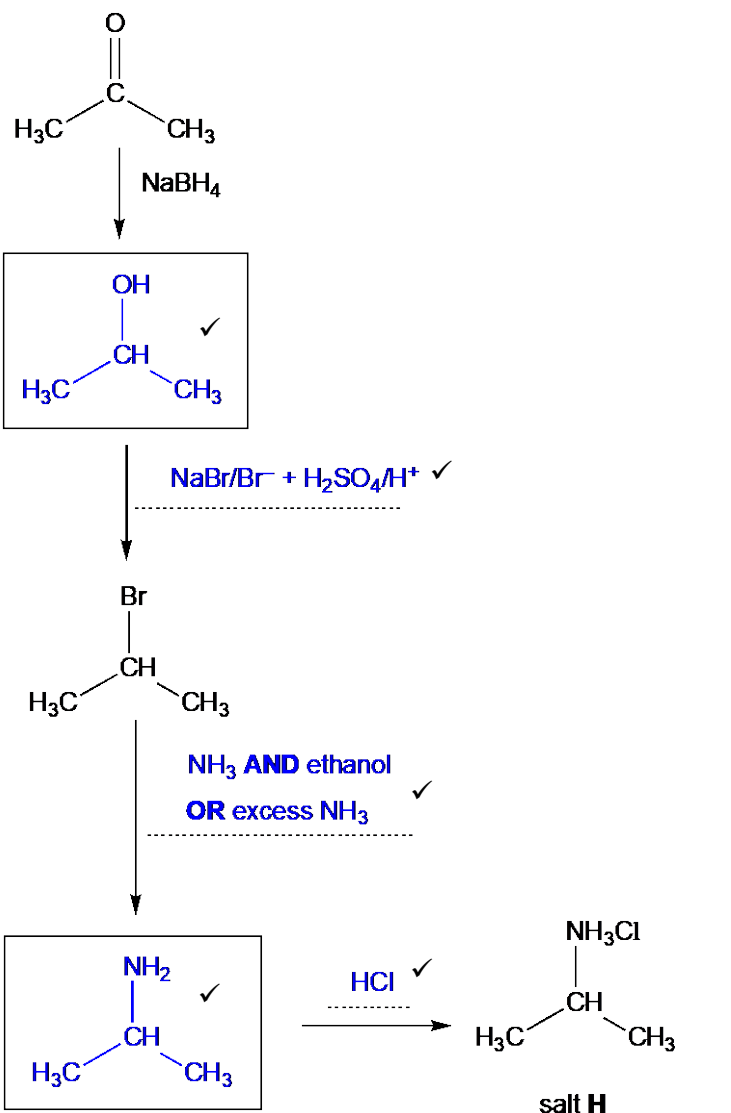
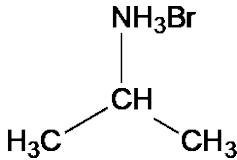


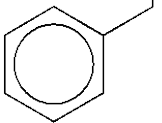
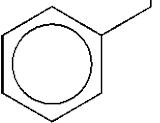
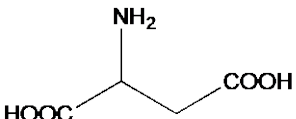
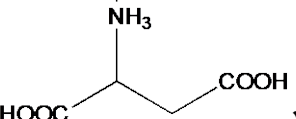
Question	Answer	Marks	AO element	Guidance
(c) (i)	<p><b>Mechanism</b> <span style="float: right;"><b>3 marks</b></span></p> <p>Curly arrow from <math>\text{CN}^-</math> to C atom of <math>\text{C}=\text{O}</math> ✓</p> <p>Dipole shown on <math>\text{C}=\text{O}</math> bond, <math>\text{C}^{\delta+}</math> and <math>\text{O}^{\delta-}</math>, <b>AND</b> curly arrow from <math>\text{C}=\text{O}</math> bond to O atom ✓</p> <p>Curly arrow from lone pair <b>OR</b> – charge on <math>\text{O}^-</math> of <b>correct</b> intermediate to <math>\text{H}^+</math> ✓</p> <hr/> <p><b>Product</b> <span style="float: right;"><b>1 mark</b></span></p> <hr/> <p><b>Name of mechanism</b> <span style="float: right;"><b>1 mark</b></span></p> <p>Nucleophilic addition ✓</p>	5	<p>1.2</p> <p>1.2</p> <p>2.5</p> <p>2.5</p> <p>1.1</p>	<p><b>ANNOTATE ANSWER WITH TICKS AND CROSSES</b></p> <p>Curly arrow must come from lone pair on C of <math>\text{CN}^-</math> <b>OR</b> <math>\text{CN}^-</math> <b>OR</b> from minus sign on C of <math>\text{CN}^-</math> ion (then lone pair on <math>\text{CN}^-</math> does not need to be shown)</p> <p>Curly arrow from <math>\text{C}=\text{O}</math> bond must start from, <b>OR</b> be traced back to, any part of <math>\text{C}=\text{O}</math> bond and go to O</p> <hr/> <p><b>ALLOW</b> curly arrow to H atom of <math>\text{H}_2\text{O}</math>, i.e.</p> <p><b>IGNORE</b> attempt to draw curly arrow showing breaking of <math>\text{H}-\text{O}</math> in <math>\text{H}_2\text{O}</math></p> <p><b>IGNORE</b> lack of dipole on <math>\text{H}_2\text{O}</math></p>

Question			Answer	Marks	AO element	Guidance
		(ii)	<b>Heterolytic</b> One (bonded) atom/O receives both/2 electrons ✓  <b>Fission</b> Breaking of a <b>covalent</b> bond ✓	2	1.2	<b>ALLOW</b> 2 electrons go to one (bonded) atom/O <b>DO NOT ALLOW</b> both pairs of electrons go to O  <b>IGNORE</b> formation of ions/radicals  For O atom, <b>ALLOW</b> species <b>DO NOT ALLOW</b> element or molecule <b>ALLOW</b> $\pi$ bond in C=O breaks  <b>IGNORE</b> breaking of C=O bond (no reference to only one bond breaking)  'Bond breaking' is <b>not</b> sufficient <i>(no reference to covalent)</i>

Question	Answer	Marks	AO element	Guidance
20 (a)*	<p><i>Refer to marking instructions on page 4 of mark scheme for guidance on marking this question.</i></p> <p><b>Level 3 (5-6 marks)</b> A correct calculation of the mass of cyclopentanol <b>AND</b> A <b>detailed</b> description of most purification steps</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><b>Level 2 (3-4 marks)</b> Calculates the mass of cyclopentanol with some errors <b>AND</b> A <b>detailed</b> description of some purification steps <b>OR</b> A correct calculation of the mass of cyclopentanol <b>AND</b> A <b>detailed</b> description of a few purification steps</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><b>Level 1 (1-2 marks)</b> Calculates the mass of cyclopentanol with some errors <b>OR</b> A <b>detailed</b> description of some purification steps</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><b>0 marks</b> No response or no response worthy of credit.</p>	6	2.8×2 3.3×4	<p><b>Indicative scientific points may include:</b> <b><u>Calculation of mass of cyclopentanol</u></b> <b>Using moles</b></p> <ul style="list-style-type: none"> <li><math>n(\text{cyclopentene}) = \frac{4.00}{68} = 0.0588\dots (\text{mol})</math></li> <li><math>n(\text{cyclopentanol}) = 0.0588 \times \frac{100}{64} = 0.0919\dots (\text{mol})</math></li> <li>Mass of cyclopentanol = <math>86 \times 0.0919 = \mathbf{7.90 \text{ g}}</math></li> </ul> <p><b>Using mass</b></p> <ul style="list-style-type: none"> <li>Theoretical mass cyclopentene = <math>4.00 \times \frac{100}{64} = 6.25 \text{ g}</math></li> <li>Theoretical <math>n(\text{cyclopentanol}) = \frac{6.25}{68} = 0.0919 (\text{mol})</math></li> <li>Mass of cyclopentanol = <math>86 \times 0.0919 = \mathbf{7.90 \text{ g}}</math></li> </ul> <p><b>ALLOW</b> for small slip in Mr / rounding errors</p> <p><b><u>Examples of some calculation errors</u></b> <b>Incorrect inverse ratio:</b></p> <ul style="list-style-type: none"> <li><math>0.0588 \times \frac{64}{100} = 0.0376\dots (\text{mol})</math></li> <li>Mass = <math>86 \times 0.0376 = 3.24 \text{ g}</math></li> </ul> <p><b>Ignoring % yield gives:</b></p> <ul style="list-style-type: none"> <li><math>\frac{4.00}{68} = 0.0588\dots (\text{mol})</math></li> <li>Mass = <math>86 \times 0.0588 = 5.06 \text{ g}</math></li> </ul> <p><b><u>Purification</u></b></p> <ul style="list-style-type: none"> <li>Add a neutralising agent <b>by formula or name</b> e.g. <math>\text{Na}_2\text{CO}_3</math></li> <li>In separating funnel, <b>organic layer is on top</b></li> <li>Drying with an <b>anhydrous salt by formula or name</b>, e.g. <math>\text{MgSO}_4</math>, <math>\text{Na}_2\text{SO}_4</math>, <math>\text{CaCl}_2</math></li> <li>Redistil <b>at approx. 44°C</b></li> </ul> <p><b>Examples of detail in bold (NOT INCLUSIVE)</b></p>

Question			Answer	Marks	AO element	Guidance
	(b)		C=C/alkene peak in region $1620-1680\text{ cm}^{-1}$ ✓ O–H/alcohol peak in region $3200-3600\text{ cm}^{-1}$ ✓	2	3.2×2	<b>LOOK ON THE SPECTRUM</b> for labelled peaks which can be given credit  <b>IGNORE</b> references to C-O at $1000\text{cm}^{-1}$

Question	Answer	Marks	AO element	Guidance
21 (a)	 <p> <math>\text{CH}_3\text{COCH}_3 \xrightarrow{\text{NaBH}_4} \text{CH}_3\text{CH(OH)CH}_3</math> ✓  <math>\text{CH}_3\text{CH(OH)CH}_3 \xrightarrow{\text{NaBr/Br}^- + \text{H}_2\text{SO}_4/\text{H}^+} \text{CH}_3\text{CH(Br)CH}_3</math> ✓  <math>\text{CH}_3\text{CH(Br)CH}_3 \xrightarrow{\text{NH}_3 \text{ AND ethanol OR excess NH}_3} \text{CH}_3\text{CH(NH}_2\text{)CH}_3</math> ✓  <math>\text{CH}_3\text{CH(NH}_2\text{)CH}_3 \xrightarrow{\text{HCl}} \text{CH}_3\text{CH(NH}_3\text{Cl)CH}_3</math> ✓            salt H         </p>	5	2.5×5	<p><b>ALLOW</b> any combination of skeletal <b>OR</b> structural <b>OR</b> displayed formula as long as unambiguous</p> <p><b>ALLOW</b> HBr</p> <p><b>ALLOW</b> for the bottom left structure</p> 

Question	Answer	Marks	AO element	Guidance
(b) (i)	Ester Amide Amine Carboxylic acid 4 groups correct ✓✓✓ 3 groups correct ✓✓ 2 groups correct ✓	3	1.2×3	<b>IGNORE</b> amino acid  <b>ALLOW</b> carboxyl  <b>IGNORE</b> attempt to classify amide, e.g. secondary <b>IGNORE</b> formulae (question asks for names)  <b>IF &gt; 4</b> functional groups are shown, • Count 4 groups max but incorrect groups <b>first</b>  <b>IGNORE</b> aryl <b>OR</b> alkyl group e.g. benzene, phenyl, aryl, arene, methyl
(ii)	<b>Methanol 1 mark</b>  $\text{H}_3\text{C}-\text{OH}$ ✓  <b>Amino Acids 3 marks</b>  <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <math>\text{HOOC}-\text{CH}(\text{NH}_2)-\text{CH}_2-\text{C}_6\text{H}_5</math>   </div> <div style="text-align: center;"> <b>OR</b>  <math>\text{HOOC}-\text{CH}(\text{NH}_3^+)-\text{CH}_2-\text{C}_6\text{H}_5</math>   </div> </div> <div style="display: flex; justify-content: space-around; align-items: center; margin-top: 20px;"> <div style="text-align: center;"> <math>\text{HOOC}-\text{CH}(\text{NH}_2)-\text{CH}_2-\text{COOH}</math>   </div> <div style="text-align: center;"> <b>OR</b>  <math>\text{HOOC}-\text{CH}(\text{NH}_3^+)-\text{CH}_2-\text{COOH}</math>   </div> </div> Both amino acids shown with $\text{NH}_3^+$ ✓	4	2.5×4	<b>ALLOW</b> any combination of skeletal <b>OR</b> structural <b>OR</b> displayed formula as long as unambiguous          <b>ALLOW</b> + charge on H of $\text{NH}_3$ group, i.e. $\text{NH}_3^+$   If <b>BOTH</b> amino acids are shown with $\text{NH}_3$ groups (without the + charge) <b>OR</b> as $\text{NH}_2^+$ groups, award 2 of the 3 marks for the amino acids  If <b>BOTH</b> amino acids are shown as correctly balanced salts, e.g. $\text{NH}_3\text{Cl}$ , all marks can be awarded.

Question			Answer	Marks	AO element	Guidance
		(iii)	<b>FIRST CHECK ANSWER ON THE ANSWER LINE</b> <b>If answer = 22.4 OR 22 OR 23 award 3 marks</b>  $n(\text{aspartame}) \text{ in 1 can} = 0.167 / 294 = 5.68 \times 10^{-4} \text{ (mol)} \checkmark$  $n(\text{aspartame}) \text{ limit per day} = 1.7 \times 10^{-4} \times 75 = 0.01275 \text{ (mol)} \checkmark$  $\text{number of cans} = 0.01275 / 5.68 \times 10^{-4} = 22.4 \checkmark$	3	2.2×3	<b>If there is an alternative answer, apply ECF and look for alternative methods</b>  <b>Alternative methods</b> $n(\text{aspartame}) \text{ in 1 can} = 0.167 / 294 = 5.68 \times 10^{-4} \text{ (mol)} \checkmark$  $n(\text{aspartame}) \text{ per kg} = 5.68 \times 10^{-4} / 75 = 7.57 \times 10^{-6} \text{ (mol)} \checkmark$  $\text{number of cans} = 1.7 \times 10^{-4} / 7.57 \times 10^{-6} = 22.4 \checkmark$  <b>OR</b>  $n(\text{aspartame}) \text{ limit per day} = 1.7 \times 10^{-4} \times 75 = 0.01275 \text{ (mol)} \checkmark$  $\text{mass(aspartame) limit per day} = 0.01275 \times 294 = 3.7485 \text{ (g)} \checkmark$  $\text{number of cans} = 3.7485 / 0.167 = 22.4 \checkmark$

Question	Answer	Marks	AO element	Guidance
22 (a)	CDCl <sub>3</sub> used as a solvent ✓  D <sub>2</sub> O used to identify OH <b>OR</b> NH protons ✓	2	1.1×2	Example and use required for each mark  <b>ALLOW</b> for 1 mark, D <sub>2</sub> O as a solvent
(b)*	<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><b>Level 3 (5–6 marks)</b> Structure <b>I</b> has a viable chemical structure of C<sub>6</sub>H<sub>9</sub>NO<sub>2</sub> which has the key features consistent with spectral data <b>AND</b> 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><b>Level 2 (3–4 marks)</b> Compound <b>I</b> has a viable chemical structure of C<sub>6</sub>H<sub>9</sub>NO<sub>2</sub> with most of the key features consistent with spectral data <b>AND</b> Some of the spectral data analysed.</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><b>Level 1 (1–2 marks)</b> Correct determination of empirical formula and/or molecular formula. <b>OR</b> Analyses some of the IR and NMR data. <b>OR</b> Analyses most of the NMR data.</p>	6	3.1× 4 3.2× 2	<p><b>Indicative scientific points:</b> <b><u>Empirical and Molecular Formulae</u></b></p> $\begin{array}{cccc} \text{C} & : & \text{H} & : & \text{N} & : & \text{O} \\ = & \frac{56.69}{12.0} & : & \frac{7.09}{1.0} & : & \frac{11.02}{14.0} & : & \frac{25.20}{16.0} \\ \text{OR} & 4.72 & : & 7.09 & : & 0.787 & : & 1.575 \\ = & 6 & : & 9 & : & 1 & : & 2 \end{array}$ <ul style="list-style-type: none"> <li>Empirical formula = C<sub>6</sub>H<sub>9</sub>NO<sub>2</sub></li> <li><i>m/z</i> = 127.0 and empirical formula mass (127) used to determine molecular formula as C<sub>6</sub>H<sub>9</sub>NO<sub>2</sub></li> </ul> <p><b><u>Structures of compound I</u></b></p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <math display="block">\begin{array}{c} \text{H} \quad \text{O} \\   \quad    \\ \text{NC}-\text{C}-\text{C}-\text{O}-\text{CH}_2\text{CH}_3 \\   \\ \text{CH}_3 \end{array}</math> </div> <div>OR</div> <div style="text-align: center;"> <math display="block">\begin{array}{c} \text{O} \quad \text{H} \\    \quad   \\ \text{CH}_3\text{CH}_2-\text{C}-\text{O}-\text{C}-\text{CN} \\   \\ \text{CH}_3 \end{array}</math> </div> </div> <p>OR</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;"> <math display="block">\begin{array}{c} \text{H} \quad \text{O} \\   \quad    \\ \text{CH}_3\text{CH}_2-\text{O}-\text{C}-\text{C}-\text{CN} \\   \\ \text{CH}_3 \end{array}</math> </div> <div>OR</div> <div style="text-align: center;"> <math display="block">\begin{array}{c} \text{O} \quad \text{H} \\    \quad   \\ \text{CH}_3\text{CH}_2-\text{C}-\text{C}-\text{O}-\text{CN} \\   \\ \text{CH}_3 \end{array}</math> </div> </div> <p><b>ALLOW</b> any combination of skeletal <b>OR</b> structural <b>OR</b> displayed formula as long as unambiguous</p>



Question	Answer	Marks	AO element	Guidance
	<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><b>0 marks</b> No response or no response worthy of credit.</p>			<p><b><u>Key features</u></b></p> <ul style="list-style-type: none"> <li>• <math>\text{C} \equiv \text{N}</math></li> <li>• <math>\text{C}=\text{O}</math> in aldehyde, ketone, ester, amide, acid anhydride</li> <li>• <math>\text{CH}_3</math> group that would give a doublet</li> <li>• <math>\text{CH}_3</math> group that would give a triplet</li> <li>• <math>\text{CH}_2</math> group that would give a quartet</li> </ul> <p><b><u><math>^1\text{H}</math> NMR and IR analysis</u></b></p> <p><math>^1\text{H}</math> NMR spectrum</p> <ul style="list-style-type: none"> <li>• <math>\delta = 4.2</math> ppm, quartet, 2H <math>\text{CH}_3\text{--CH}_2\text{--O}</math></li> <li>• <math>\delta = 2.9</math> ppm, quartet, 1H <math>\text{CO--CH--CH}_3</math></li> <li>• <math>\delta = 1.7</math> ppm, doublet, 3H <math>\text{CO--CH--CH}_3</math></li> <li>• <math>\delta = 1.3</math> ppm, triplet, 3H <math>\text{CH}_3\text{--CH}_2</math></li> </ul> <p>IR spectrum</p> <ul style="list-style-type: none"> <li>• peak at <math>1750\text{ (cm}^{-1}\text{)}</math> is <math>\text{C}=\text{O}</math></li> <li>• peak at <math>2280\text{ (cm}^{-1}\text{)}</math> is <math>\text{C} \equiv \text{N}</math></li> </ul> <p><b>ALLOW</b> ranges from <i>Data Sheet</i>  <b>IGNORE</b> references to <math>\text{C--O}</math> peaks</p>

**OCR (Oxford Cambridge and RSA Examinations)**  
**The Triangle Building**  
**Shaftesbury Road**  
**Cambridge**  
**CB2 8EA**

**OCR Customer Contact Centre**

**Education and Learning**

Telephone: 01223 553998

Facsimile: 01223 552627

Email: [general.qualifications@ocr.org.uk](mailto:general.qualifications@ocr.org.uk)

[www.ocr.org.uk](http://www.ocr.org.uk)

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