

GCE

Chemistry A

Unit **H432A/02**: Synthesis and analytical techniques

Advanced GCE

Mark Scheme for June 2017

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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.

OCR will not enter into any discussion or correspondence in connection with this mark scheme.

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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

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

Annotation	Meaning
/	alternative and acceptable answers for the same marking point
✓	Separates marking points
DO NOT ALLOW	Answers which are not worthy of credit
IGNORE	Statements which are irrelevant
ALLOW	Answers that can be accepted
()	Words which are not essential to gain credit
—	Underlined words must be present in answer to score a mark
ECF	Error carried forward
AW	Alternative wording
ORA	Or reverse argument

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.

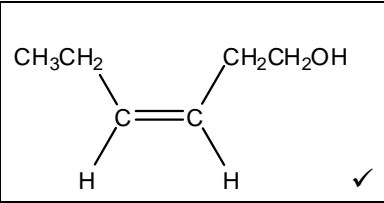
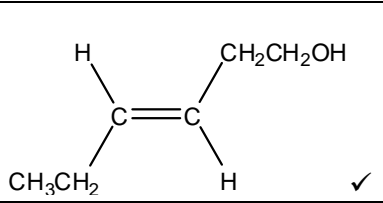
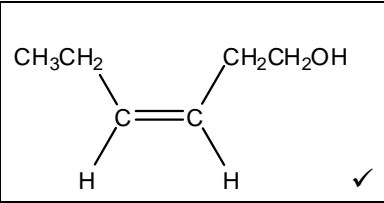
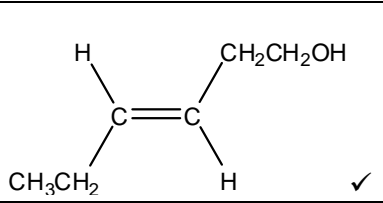
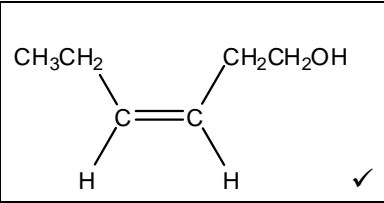
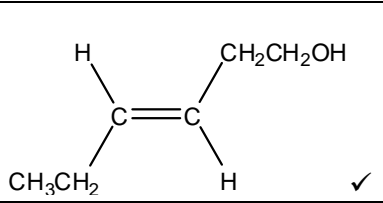
You should ensure that you have copies of these materials.

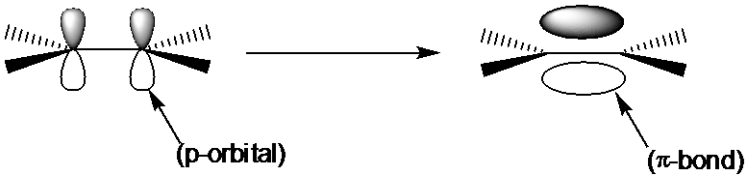
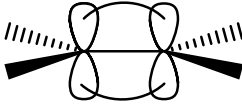
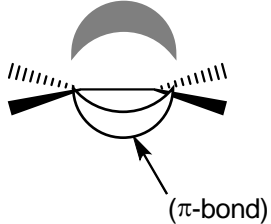
You should ensure also that you are familiar with the administrative procedures related to the marking process. These are set out in the OCR booklet **Instructions for Examiners**. If you are examining for the first time, please read carefully **Appendix 5 Introduction to Script Marking: Notes for New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

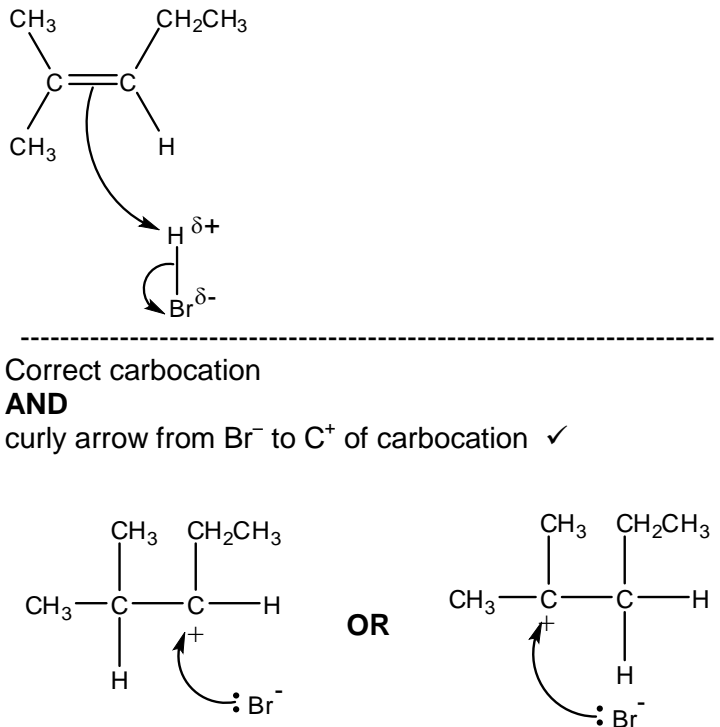
Please ask for help or guidance whenever you need it. Your first point of contact is your Team Leader.

Question	Key	Marks	Guidance
1	B	1	
2	D	1	
3	C	1	
4	B	1	
5	D	1	
6	C	1	ALLOW 3 (This is the trigonal planar atom)
7	A	1	
8	C	1	ALLOW 4 (This is the number of chiral centres)
9	C	1	
10	D	1	
11	C	1	ALLOW 3 (This is the number of peaks in the NMR spectrum)
12	A	1	
13	A	1	
14	C	1	
15	A	1	

Question		Answer	Marks	Guidance	
16	(a)	<p>Compound A (is branched so) has less points of contact / less surface interaction between molecules ✓</p> <p>Induced dipole–dipole interactions / London (dispersion) forces are weaker. AND Require less energy to break (these interactions / forces) ✓</p>	2	<p>Both answers need to be comparisons ALLOW ORA throughout</p> <p>DO NOT ALLOW ‘more contact between atoms’</p> <p>IGNORE van der Waals’ forces/VDW for induced dipole–dipole interactions (ambiguous as this term refers to both permanent dipole – dipole and induced dipole–dipole forces)</p> <p>ALLOW fewer induced dipole-dipole interactions.</p> <p>IGNORE it is easier to break the induced dipole-dipole / London forces. (reference to energy required) IGNORE less energy required to separate molecules IGNORE less energy is needed to break the bonds.</p>	
	(b)	(i)	Hex-3-en-1-ol ✓	1	<p>ALLOW Hex-3-ene-1-ol</p> <p>ALLOW 1-hydroxyhex-3-ene as this is unambiguous</p> <p>Hex-3-enol is not sufficient</p> <p>IGNORE lack of hyphens, or addition of commas</p>

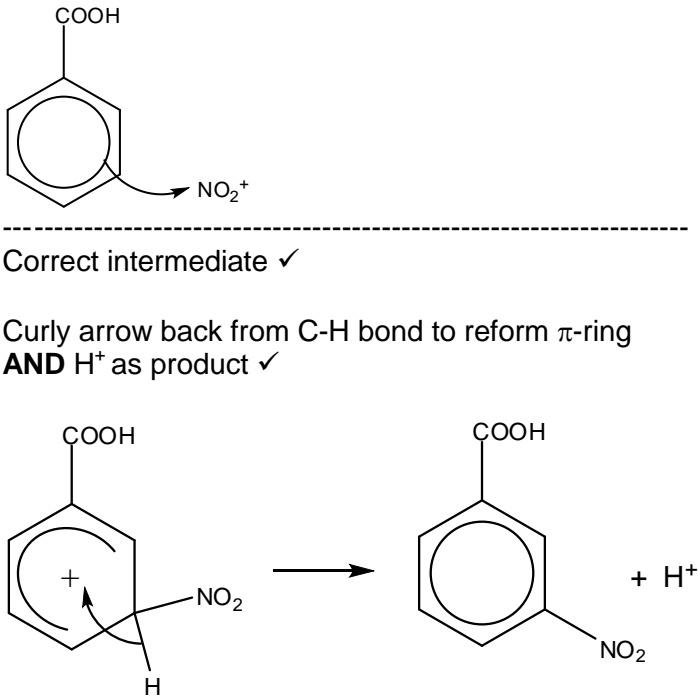
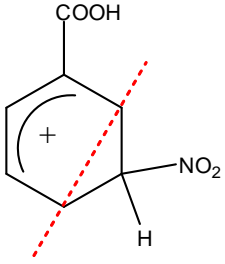
Question	Answer	Marks	Guidance				
(ii)	Same structural formula AND Different arrangement (of atoms) in space OR different spatial arrangement (of atoms) ✓	1	ALLOW have the same structure/displayed formula/skeletal formula DO NOT ALLOW same empirical formula OR same general formula IGNORE same molecular formula Reference to <i>E/Z</i> isomerism or optical isomerism is not sufficient				
(iii)	<table border="1" style="width: 100%; border-collapse: collapse;"> <tbody> <tr> <td style="text-align: center; padding: 10px;">  </td> <td style="text-align: center; padding: 10px;">  </td> </tr> <tr> <td style="text-align: center; padding: 5px;"><i>cis</i></td> <td style="text-align: center; padding: 5px;"><i>trans</i></td> </tr> </tbody> </table>			<i>cis</i>	<i>trans</i>	2	ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous ALLOW one mark if both stereoisomers of compound C are shown but in the incorrect columns ALLOW one mark for correct stereoisomers of compound C in correct columns where – CH ₂ CH ₂ OH is represented as –C ₂ H ₅ O or –C ₂ H ₄ OH DO NOT ALLOW incorrect connectivity e.g. –CH ₃ CH ₂ on first occasion but allow ECF in second structure.
							
<i>cis</i>	<i>trans</i>						

Question	Answer	Marks	Guidance
(c)	 <p>Two p-orbitals shown as a “dumb-bell” added to structure on left.</p> <p>AND</p> <p>π-bond on structure on right ✓</p>	1	<p>DO NOT ALLOW C=C in diagram</p> <p>DO NOT ALLOW overlapping p orbitals on left hand side in the diagram.</p> <p>DO NOT ALLOW a diagram that contains four lobes on the right hand side.</p> <p>e.g. </p> <p>IGNORE any atoms joined to the bonds</p> <p>Note: labels are not required</p> <p>ALLOW the following diagram to show the π-bond</p> 
(d)	(i)	1	
	(ii)	2	<p>ALLOW correct structural OR displayed OR skeletal formulae OR a combination of above as long as unambiguous</p> <p>ALLOW in either order</p>

Question	Answer	Marks	Guidance
(iii)	<p>Curly arrow from C=C bond to H of H-Br ✓</p> <p>Correct dipole shown on H-Br AND curly arrow showing the breaking of H-Br bond ✓</p>  <p>-----</p> <p>Correct carbocation AND curly arrow from Br⁻ to C⁺ of carbocation ✓</p>	3	<p>ANNOTATE ANSWER WITH TICKS AND CROSSES</p> <p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>DO NOT ALLOW partial charges shown on C=C double bond (the second marking point)</p> <p>DO NOT ALLOW $\delta+$ on C of carbocation</p> <p>Curly arrow must come from a lone pair on Br⁻ OR from the negative sign of Br⁻ ion (then lone pair on Br⁻ ion does not need to be shown)</p>

Question	Answer	Marks	Guidance
	<p>(iv)</p> $ \begin{array}{c} \text{CH}_3 \quad \text{CH}_2\text{CH}_3 \\ \quad \\ \text{H}_3\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{Br} \quad \text{H} \end{array} $ <p>2-bromo-2-methylpentane</p> <p>AND</p> <p>(the) carbocation intermediate (in the formation of 2-bromo-2-methylpentane) is more stable (than the carbocation in the formation of the other product) ✓</p>	1	<p>Note: the correct product and explanation are both required for the mark</p> <p>The major product may be identified by its</p> <ul style="list-style-type: none"> • corresponding letter (E or F) from the table in (d)(ii) • correct structure • correct name <p>DO NOT ALLOW product comes from the more stable secondary or primary carbocation</p> <p>IGNORE explanations based on Markownikoff's rule.</p>
(e)	<p>(i)</p> $n(\text{myrcene}) = \frac{204 \times 10^{-3}}{136.0} = 1.5(0) \times 10^{-3} \text{ (mol) } \checkmark$ $ \begin{aligned} \text{Volume of H}_2 &= 3 \times 1.5(0) \times 10^{-3} \times 24000 \\ &= 108 \text{ (cm}^3\text{)} \checkmark \end{aligned} $	2	<p>Correct working required for the first marking point.</p> <p>ALLOW ECF from incorrect moles of myrcene i.e. $n(\text{myrcene}) \times 3 \times 24000$</p> <p>Common incorrect answers</p> <p>108000 cm³ = 1 mark (not converted to g) 12cm³ = 1 mark (divided by 3) 36 cm³ = 1 mark (not multiplied by 3)</p> <p>IGNORE Calculations based on $pV = nRT$</p>

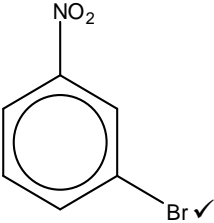
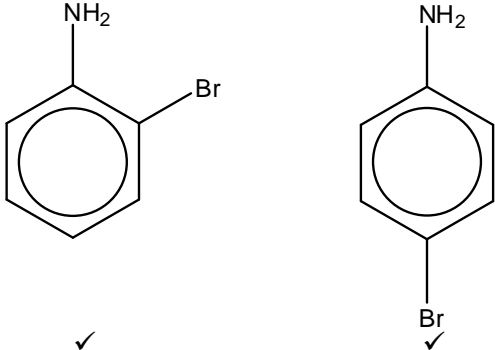
Question	Answer	Marks	Guidance
(ii)	<p>Amount of hydrogen</p> $n(\text{H}_2) = \frac{5.28}{24.0} = 0.22(0) \text{ (mol)} \quad \checkmark$ <p>Number of double bonds</p> $= \frac{0.220}{0.0200} = 11 \quad \checkmark$ <p>Formula of saturated product</p> $\text{C}_{40}\text{H}_{78} \quad \checkmark$ <p>Equation</p> $\text{C}_{40}\text{H}_{56} + 11\text{H}_2 \longrightarrow \text{C}_{40}\text{H}_{78} \quad \checkmark$	4	<p>ALLOW Evidence of $n(\text{H}_2) = \frac{5.28}{24.0}$ if 0.22 is not seen</p> <p>Evidence for 11 double bonds could come from 11H_2 in equation</p> <p>Formula could be shown as the product of an equation</p> <p>ALLOW ECF from $\text{C}_{40}\text{H}_{82}$ and $\text{C}_{40}\text{H}_{80}$ only i.e. $\text{C}_{40}\text{H}_{60} + 11\text{H}_2 \longrightarrow \text{C}_{40}\text{H}_{82}$ $\text{C}_{40}\text{H}_{58} + 11\text{H}_2 \longrightarrow \text{C}_{40}\text{H}_{80}$</p>
	Total	20	

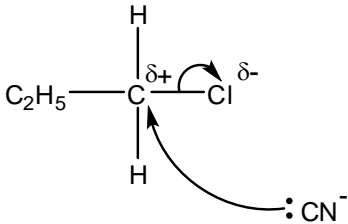
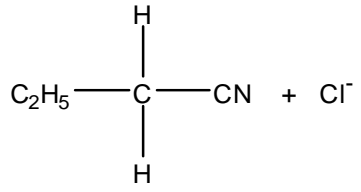
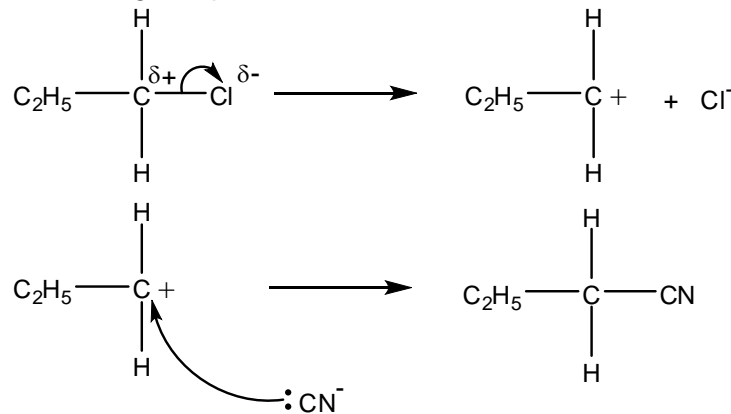
Question	Answer	Marks	Guidance
17 (a) (i)	<p>Generation of electrophile</p> $\text{HNO}_3 + \text{H}_2\text{SO}_4 \longrightarrow \text{H}_2\text{O} + \text{HSO}_4^- + \text{NO}_2^+ \checkmark$ <p>Electrophilic substitution</p> <p>Curly arrow from π-bond to NO_2^+ \checkmark</p>  <p>Correct intermediate \checkmark</p> <p>Curly arrow back from C-H bond to reform π-ring AND H^+ as product \checkmark</p> <p>Regeneration of catalyst</p> $\text{H}^+ + \text{HSO}_4^- \longrightarrow \text{H}_2\text{SO}_4 \checkmark$	5	<p>ANNOTATE ANSWER WITH TICKS AND CROSSES</p> <p>ALLOW $\text{HNO}_3 + 2\text{H}_2\text{SO}_4 \rightarrow \text{H}_3\text{O}^+ + 2\text{HSO}_4^- + \text{NO}_2^+$</p> <p>ALLOW $\text{HNO}_3 + \text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{NO}_3^+ + \text{HSO}_4^-$ then $\text{H}_2\text{NO}_3^+ \rightarrow \text{H}_2\text{O} + \text{NO}_2^+$</p> <p>ALLOW $^+\text{NO}_2$ OR NO_2^+</p> <p>First curly arrow must come from the ring to NO_2^+</p> <p>DO NOT ALLOW the following intermediate:</p>  <p>π-ring should cover approximately 4 of the 6 sides of the benzene ring structure AND the correct orientation, <i>i.e.</i> gap towards C with NO_2</p> <p>ALLOW + sign anywhere inside the 'hexagon' of intermediate</p>

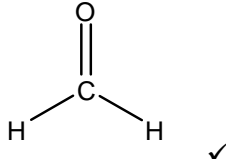
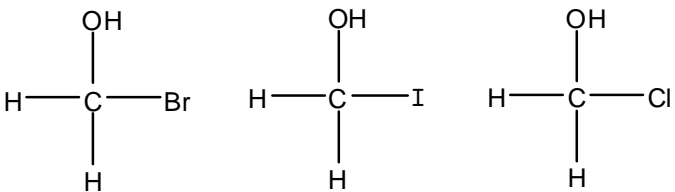
Question	Answer	Marks	Guidance
	<p>(ii)* <i>Please refer to the marking instructions on page 5 of this mark scheme for guidance on how to mark this question.</i></p> <p>Level 3 (5–6 marks)</p> <p>Outlines the main steps of recrystallisation to produce a pure sample of 3-nitrobenzoic acid from the impure solid. AND Calculates correct percentage yield of 3-nitrobenzoic acid. AND Method of checking purity to include comparison to relevant data.</p> <p><i>A well-structured response with the steps for recrystallisation and the determination of purity being given in the correct order. Correct use of terminology throughout.</i></p> <p>Level 2 (3–4 marks)</p> <p>Attempts all three scientific points but explanations may be incomplete. OR Explains two scientific points thoroughly with very few omissions.</p> <p><i>The description of checking for purity or recrystallisation is clear and any calculations structured. Key terminology used appropriately.</i></p> <p>Level 1 (1–2 marks)</p> <p>A simple explanation based on at least two of the main scientific points. OR</p>	6	<p>Indicative scientific points, with bulleted elements, may include:</p> <p>1. Purification</p> <ul style="list-style-type: none"> Recrystallisation Dissolve impure solid in minimum volume of hot water/solvent Cool solution and filter solid Wash with cold water/solvent and dry <p>2. Percentage yield</p> <ul style="list-style-type: none"> $n(\text{benzoic acid}) \text{ used} = \frac{4.97}{122} = 0.0407 \text{ (mol)}$ $n(3\text{-nitrobenzoic acid}) \text{ made} = \frac{4.85}{167} = 0.0290 \text{ (mol)}$ $\text{percentage yield} = \frac{0.0290}{0.0407} \times 100 = 71.3 \text{ (\%)}$ <p>ALLOW 71 to calculator value of 71.29001554 correctly rounded.</p> <p>CHECK for extent of errors by ECF</p> <p>Alternative correct calculation may calculate theoretical mass of 3-nitrobenzoic acid that can be produced as $0.0407 \times 167 = 6.80 \text{ (g)}$ followed by:</p> $\text{percentage yield} = \frac{4.85}{6.80} \times 100 = 71.3 \text{ (\%)}$ <p>Calculation must attempt to calculate $n(\text{benzoic acid})$ in mol.</p> <p>3. Checking purity</p>

Question		Answer	Marks	Guidance
		<p>Explains one scientific point thoroughly with few omissions.</p> <p><i>There is an attempt at a logical structure. The description of the practical techniques provides some detail but may not be in the correct order.</i></p> <ul style="list-style-type: none"> <i>Purification step is unclear with few scientific terms and little detail, e.g. just 'recrystallise'.</i> <i>Calculation is difficult to follow, may just include a calculation of moles of reactants and/or products.</i> <i>Purity check specifies a method but this is unclear with little detail, e.g. take melting point.</i> <p>0 marks No response or no response worthy of credit.</p>		<ul style="list-style-type: none"> Obtain melting point Compare to known values Pure sample will have a (sharp) melting point very close to data book value <p>ALLOW alternative approach based on spectroscopy or TLC</p> <p>Spectroscopy</p> <ul style="list-style-type: none"> Run an NMR/IR spectrum Compare to (spectral) database Spectrum of pure sample will contain same peaks and not others <p>TLC</p> <ul style="list-style-type: none"> Run a TLC Compare (R_f value) to known data Pure sample will have a very similar R_f
(b)	(i)	<p>Phenol is the most easily nitrated/ most reactive AND Benzoic acid is the least easily nitrated /least reactive ✓</p>	1	<p>Response must give rank order of reactivity</p> <p>e.g. nitration becomes more difficult from phenol (to benzene) to benzoic acid</p> <p>OR nitration becomes easier from right to left in the table</p>
	(ii)	<p>Reactivity of phenol</p> <p>a (lone) pair of electrons on O is (partially) delocalised/donated into the π-system / ring ✓</p>	3	<p>ANNOTATE ANSWER WITH TICKS AND CROSSES</p> <p>ALLOW the electron pair in the p orbitals of the O atom becomes part of the π-system / ring</p> <p>ALLOW diagram to show movement of lone pair into ring</p>

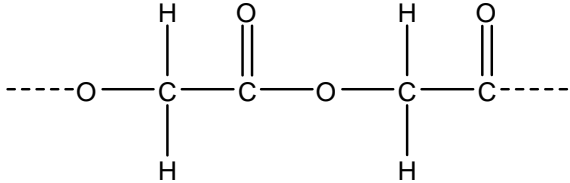
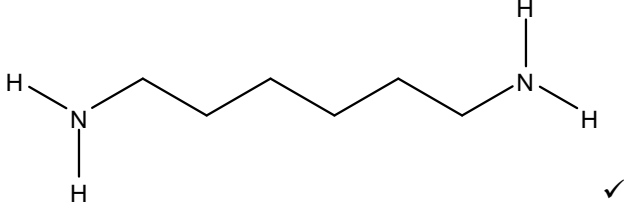
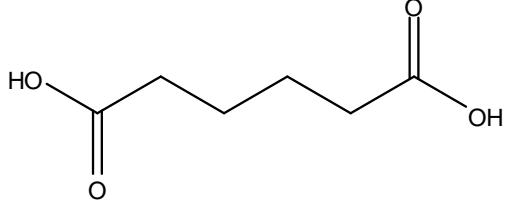
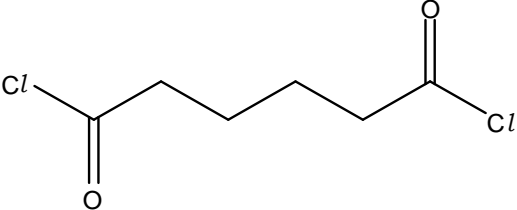
Question		Answer	Marks	Guidance
		<p>Reactivity of benzoic acid</p> <p>The –COOH group on benzoic acid is an electron withdrawing group ✓</p> <p>Links electron density in π-bond to reactivity</p> <p>In phenol electron density is higher AND The ring is more susceptible to attack</p> <p>OR</p> <p>In benzoic acid electron density is lower AND The ring is less susceptible to attack ✓</p>		<p>ALLOW lone pair of electrons on O is (partially) drawn/attracted/pulled into π-system / ring</p> <p>IGNORE activating and deactivating.</p> <p>ALLOW the following alternatives for susceptibility to attack:</p> <ul style="list-style-type: none"> • phenol attracts electrophiles / NO_2^+ more • phenol polarises electrophiles / NO_2^+ more • benzoic acid attracts electrophiles / NO_2^+ less • benzoic acid polarises electrophiles / NO_2^+ less
	(c) (i)	<p>Bromination: Br_2 AND $\text{AlBr}_3/\text{FeBr}_3/\text{Fe}$ ✓</p> <p>Intermediate</p>	3	<p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>ALLOW any suitable halogen carrier catalyst</p>

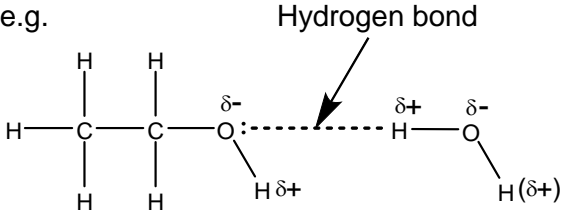
Question	Answer	Marks	Guidance
	 <p>Reduction: Sn AND (concentrated) HCl ✓</p>		<p>ALLOW Kekulé structure</p> <p>IGNORE names (<i>question asks for formulae</i>)</p> <p>IGNORE reaction conditions even if incorrect</p> <p>IGNORE 'dilute' for HCl</p> <p>IGNORE H₂</p> <p>IGNORE NaOH if seen as a reagent to convert nitro group into amine e.g 'Sn/(concentrated) HCl then NaOH' scores the mark</p>
(ii)	<p>NH₂ is 2,4 directing ✓</p> <p>Products (1 mark for each):</p> 	3	<p>IGNORE references to electron donating/withdrawing groups</p> <p>ALLOW –NH₂ activates the ring causing the new group to join at positions 2 and 4.</p> <p>ALLOW ortho and para directing for 2,4 directing</p> <p>IGNORE 6-directing</p> <p>ALLOW Kekulé structure</p> <p>IGNORE names</p>
	Total	21	

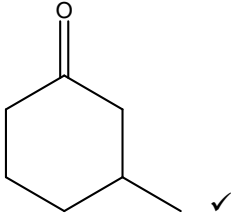
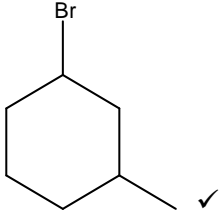
Question	Answer	Marks	Guidance
18	<p>(a) (i) curly arrow from CN^- to carbon atom of $\text{C}-\text{Cl}$ bond ✓</p> <p>Dipole shown on $\text{C}-\text{Cl}$ bond, $\text{C}^{\delta+}$ and $\text{Cl}^{\delta-}$, AND curly arrow from $\text{C}-\text{Cl}$ bond to Cl atom ✓</p>  <p>-----</p> <p>correct organic product AND Cl^- ✓</p> 	3	<p>ANNOTATE ANSWER WITH TICKS AND CROSSES</p> <p>Curly arrow must come from lone pair on C of CN^- OR CN^- OR from minus sign on C of CN^- ion (then lone pair on CN^- does not need to be shown)</p> <p>IGNORE NaCl</p> <p>-----</p> <p>ALLOW $\text{S}_{\text{N}}1$ mechanism:</p> <p>Dipole shown on $\text{C}-\text{Cl}$ bond, $\text{C}^{\delta+}$ and $\text{Cl}^{\delta-}$, AND curly arrow from $\text{C}-\text{Cl}$ bond to Cl atom ✓</p> <p>Correct carbocation AND curly arrow from CN^- to carbocation. Curly arrow must come from lone pair on C of CN^- OR CN^- OR from minus sign on C of CN^- ion (then lone pair on CN^- does not need to be shown) ✓</p> <p>correct organic product AND Cl^- ✓</p> 

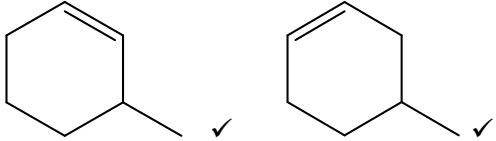
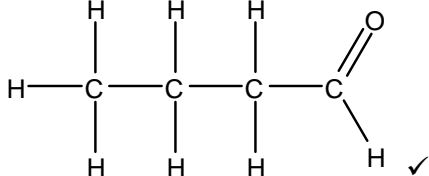
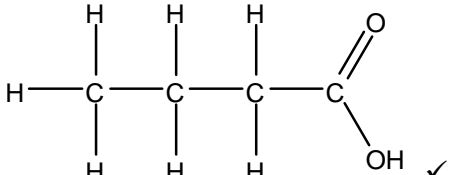
Question	Answer	Marks	Guidance
(ii)	<p>Compound G</p>  <p>Reagents</p> <p>Reaction 2: H₂ AND Ni ✓</p> <p>Reaction 3: Correct formula of an aqueous acid e.g. HCl(aq)/H₂SO₄(aq) ✓</p>	3	<p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>IGNORE name(s)</p> <p>ALLOW</p>  <p>ALLOW any suitable metal catalyst e.g. Pt ALLOW LiAlH₄ for reagent in reaction 2 DO NOT ALLOW NaBH₄ for reagent in reaction 2 IGNORE names (<i>question asks for formulae</i>)</p> <p>IGNORE references to temperature and/or pressure</p> <p>ALLOW H⁺(aq) IGNORE dilute ALLOW formula of an acid AND water e.g. HCl AND H₂O H₂SO₄ AND H₂O</p>

Question	Answer	Marks	Guidance
(iii)	<p>Explanation</p> <p>Nitrogen electron pair OR nitrogen lone pair AND accepts a proton/H⁺ ✓</p> <p>Structure of salt</p> $ \begin{array}{c} \text{OH} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{NH}_3^+ \\ \quad \\ \text{H} \quad \text{H} \end{array} $ <p>AND Cl⁻ ✓</p>	2	<p>IGNORE NH₂ group donates electron pair</p> <p>ALLOW nitrogen donates an electron pair to H⁺ DO NOT ALLOW nitrogen donates lone pair to acid IGNORE comments about the O in the –OH group</p> <p>Compound H is a base is not sufficient (<i>role of lone pair required</i>)</p> <p>DO NOT ALLOW nitrogen/N lone pair accepts hydrogen (<i>proton/H⁺ required</i>)</p> <p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>ALLOW</p> $ \begin{array}{c} \text{OH} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{NH}_3\text{Cl} \\ \quad \\ \text{H} \quad \text{H} \end{array} $ <p><i>i.e.</i> charges not required</p> <p>IF charges are shown both need to be present</p> <p>ALLOW charge either on N atom or NH₃⁺</p> <p>IF displayed then + charge must be on the nitrogen</p>

Question	Answer	Marks	Guidance
(iv)	 <p>Ester link ✓</p> <p>Rest of structure ✓</p> <p>(polymer J is biodegradable because) the ester / ester bond / ester group / polyester can be hydrolysed ✓</p>	3	<p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>DO NOT ALLOW more than two repeat units for second marking point.</p> <p>'End bonds' MUST be shown (do not have to be dotted)</p> <p>IGNORE brackets</p> <p>IGNORE <i>n</i></p> <p>Broken down by water is not sufficient</p> <p>IGNORE references to photodegradable</p>
(b) (i)	 ✓  ✓	2	<p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>ALLOW</p> 
(ii)	$(n = \frac{21500}{226} =) 95 \text{ (repeat units)}$	1	<p>MUST be a whole number.</p> <p>DO NOT ALLOW an answer that uses an incorrect molar mass in the working.</p> <p>ALLOW 96</p>
Total	14		

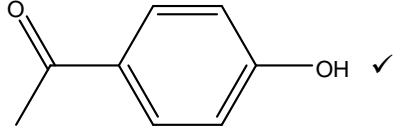
Question	Answer	Marks	Guidance
19 (a)	$\text{C}_5\text{H}_{10}\text{O} + 7\text{O}_2 \longrightarrow 5\text{CO}_2 + 5\text{H}_2\text{O} \checkmark$	1	<p>ALLOW multiples</p> <p>e.g. $2\text{C}_5\text{H}_{10}\text{O} + 14\text{O}_2 \longrightarrow 10\text{CO}_2 + 10\text{H}_2\text{O}$</p> <p>ALLOW any equation involving an unsaturated alcohol with correct balancing</p> <p>e.g.</p> $\text{C}_5\text{H}_8\text{O} + 6.5\text{O}_2 \longrightarrow 5\text{CO}_2 + 4\text{H}_2\text{O}$ $\text{C}_5\text{H}_6\text{O} + 6\text{O}_2 \longrightarrow 5\text{CO}_2 + 3\text{H}_2\text{O}$ $\text{C}_5\text{H}_4\text{O} + 5.5\text{O}_2 \longrightarrow 5\text{CO}_2 + 2\text{H}_2\text{O}$ $\text{C}_5\text{H}_2\text{O} + 5\text{O}_2 \longrightarrow 5\text{CO}_2 + \text{H}_2\text{O}$ <p>IGNORE state symbols</p>
(b) (i)	<p>Diagram showing a water molecule and an ethanol molecule with at least one $\text{H}^{\delta+}$ and one $\text{O}^{\delta-}$ on BOTH molecules \checkmark</p> <p>Hydrogen bond between one lone pair on O atom in one of the molecules and the H atom of another.</p> <p>AND</p> <p>Hydrogen bonding stated or labelled on diagram \checkmark</p> <p>e.g.</p> 	2	<p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>DO NOT ALLOW $\delta+$ on H atoms of alkyl group</p> <p>DO NOT ALLOW any marks for a diagram containing O_2H</p> <p>If more than one hydrogen bond is shown they must all be correct to award the mark.</p>

Question	Answer	Marks	Guidance
	<p>(ii) Hexane-1,6-diol has more OH groups (than hexan-1-ol)</p> <p>AND</p> <p>(hexane-1,6-diol) forms more hydrogen bonds with water</p> <p>✓</p>	1	<p>Statements MUST be comparative</p> <p>e.g. hexane-1,6-diol has two –OH groups and hexan-1-ol has one -OH group</p> <p>ALLOW hydroxyl or hydroxy</p> <p>DO NOT ALLOW hydroxide/OH⁻</p> <p>ALLOW ORA</p>
(c)	<p>(i) Starting material from reduction reaction</p>  <p>Reagent for reduction</p> <p>NaBH₄ ✓</p> <p>Product from reaction with NaBr/H₂SO₄</p>  <p>Structural isomers</p>	5	<p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>Watch for missing methyl groups</p> <p>IGNORE H⁺ / acid or H₂O or ethanol</p> <p>ALLOW sodium borohydride</p> <p>OR sodium tetrahydridoborate</p> <p>ALLOW LiAlH₄</p>

Question	Answer	Marks	Guidance
			<p>ALLOW in either order</p>
(ii)	3-methylcyclohexanol ✓	1	<p>ALLOW 3-methylcyclohexan-1-ol ALLOW 1-methylcyclohexan-3-ol IGNORE lack of hyphens, or addition of commas</p>
(d)	<p>Structures of organic products</p>   <p>Equations</p> $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH} + [\text{O}] \longrightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} + \text{H}_2\text{O}$ <p>✓</p> $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH} + 2[\text{O}] \longrightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{COOH} + \text{H}_2\text{O}$ <p>✓</p> <p>Reaction conditions</p>	5	<p>ANNOTATE WITH TICKS AND CROSSES</p> <p>Use of any primary alcohol containing 3, 5 or more carbons can be awarded up to 4 marks.</p> <p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p> <p>IGNORE names</p> <p>DO NOT ALLOW $\text{CH}_3\text{CH}_2\text{CH}_2\text{COH}$ for the structure of the aldehyde.</p> <p>ALLOW $\text{CH}_3\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$ for the structure of the carboxylic acid.</p> <p>ALLOW marks for structures from equations as long as unambiguous. ALLOW molecular formulae in equations e.g. $\text{C}_4\text{H}_{10}\text{O} + [\text{O}] \longrightarrow \text{C}_4\text{H}_8\text{O} + \text{H}_2\text{O}$ $\text{C}_4\text{H}_{10}\text{O} + 2[\text{O}] \longrightarrow \text{C}_4\text{H}_8\text{O}_2 + \text{H}_2\text{O}$ $\text{C}_4\text{H}_9\text{OH} + [\text{O}] \longrightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O}$ $\text{C}_4\text{H}_9\text{OH} + 2[\text{O}] \longrightarrow \text{C}_3\text{H}_7\text{CO}_2\text{H} + \text{H}_2\text{O}$</p> <p>IGNORE incorrect structures in equations i.e. $\text{C}_4\text{H}_{10}\text{O} + [\text{O}] \longrightarrow \text{C}_3\text{H}_7\text{COH} + \text{H}_2\text{O}$</p>

Question		Answer	Marks	Guidance
		Distillation to produce aldehyde/ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$ AND Reflux to produce carboxylic acid/ $\text{CH}_3\text{CH}_2\text{CH}_2\text{COOH}$ ✓		scores equation mark Conditions must be linked to aldehyde/carboxylic acid or correct products. Conditions may be written above arrow of equation.
Total			15	

Question		Answer	Marks	Guidance
20	(a)	Empirical formula Mole Ratio C : H : O = 5.88 : 5.92 : 1.47 ✓ Empirical formula = $\text{C}_4\text{H}_4\text{O}$ ✓ Molecular formula Molecular formula = $\text{C}_8\text{H}_8\text{O}_2$ AND Evidence of 136 in working or from labelled peak in spectrum ✓	3	ANNOTATE ANSWER WITH TICKS AND CROSSES ALLOW $\frac{70.58}{12.0} : \frac{5.92}{1.0} : \frac{23.50}{16.0}$ ALLOW 4:4:1 if linked to C:H:O Alternative method for 3 marks: C: $\frac{136 \times 70.58/100}{12.0} = 8$ H: $\frac{136 \times 5.92/100}{1.0} = 8$ O: $\frac{136 \times 23.50/100}{16.0} = 2$
	(b)	Functional groups Phenol AND ketone ✓ Explanation	3	DO NOT ALLOW any other functional groups for first marking point.

Question	Answer	Marks	Guidance
	Links phenol to (weak) acidity AND no reaction with Na ₂ CO ₃ (so not carboxylic acid) ✓ Links 2,4-DNP(H) or Brady's reagent observation to carbonyl AND Tollens' reagent observation (so not an aldehyde) ✓		ALLOW identity of functional groups in the explanation if not stated on functional group prompt line. ALLOW "aldehyde or ketone" in place of carbonyl
(c)	Carbon NMR analysis Peaks between 110–160 ppm are the (four) aromatic (carbon environments) ✓ Compound contains a C=O between 190 - 200 ppm AND Compound contains a C-C at 20-30 ppm ✓ Structure 	3	ALLOW peaks to be identified by: <ul style="list-style-type: none"> • Peaks labelled on spectrum • Peaks indicated on a chemical structure • Peaks indicated from within text Note: If identifying aromatic peaks from the spectrum all four peaks should be indicated. ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous
	Total	9	

Question	Answer	Marks	Guidance
21*	<p><i>Please refer to the marking instructions on page 5 of this mark scheme for guidance on how to mark this question.</i></p> <p>Level 3 (5–6 marks) Structure of L is $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{C}(\text{CH}_3)_3$ OR $(\text{CH}_3)_3\text{CCH}_2\text{COOCH}_2\text{CH}_3$ AND A comprehensive explanation with most of the spectral data analysed and few omissions. <i>There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.</i> <i>Splitting patterns used to deduce the correct structure of L.</i></p> <p>Level 2 (3–4 marks) Attempts all three scientific points but explanations may be incomplete and/or structure of L incorrect. OR Explains two scientific points thoroughly with few omissions. <i>There is a line of reasoning presented with some structure. The information presented in the most part relevant and supported by some evidence.</i> <i>The analysis is clear and includes some interpretation of NMR/IR peaks.</i></p> <p>Level 1 (1–2 marks) A simple explanation based on at least two of the main scientific points. OR Explains one scientific point thoroughly with few omissions. <i>There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.</i></p>	6	<p>Indicative scientific points may include:</p> <p>1. ¹H NMR spectrum</p> <ul style="list-style-type: none"> • $\delta = 1.1$ ppm, triplet, 3H $\text{CH}_3\text{--CH}_2\text{--}$ • $\delta = 1.3$ ppm, singlet, 9H $(\text{CH}_3)_3\text{C--}$ • $\delta = 2.3$ ppm, quartet, 2H $\text{CH}_3\text{--CH}_2\text{--C=O}$ • $\delta = 4.0$ ppm, singlet, 2H $\text{--CH}_2\text{--O--}$ <p>ALLOW approximate values for chemical shifts.</p> <p>2. Infrared spectra IR spectrum of M</p> <ul style="list-style-type: none"> • peak at 2300–3700 (cm^{-1}) is O–H • peak at ~1720 (cm^{-1}) is C=O • M is a carboxylic acid <p>IR spectrum of N</p> <ul style="list-style-type: none"> • peak at 3100-3700 (cm^{-1}) is O–H • N is an alcohol <p>ALLOW ranges from <i>Data Sheet</i> IGNORE references to C–O peaks</p> <p>3. Structure of L</p> <ul style="list-style-type: none"> • L is an ester (as it reacts with $\text{HCl}(\text{aq})$ to form carboxylic acid and alcohol)

Question	Answer	Marks	Guidance
	<p><i>The analysis is communicated in an unstructured way and includes interpretation of a few peaks from the NMR/IR spectra.</i></p> <p>0 marks No response or no response worthy of credit.</p>		<ul style="list-style-type: none"> • Correct structure $ \begin{array}{ccccccc} & \text{H} & \text{H} & \text{O} & & \text{H} & \text{CH}_3 \\ & & & & & & \\ \text{H} & - \text{C} & - \text{C} & - \text{C} & - \text{O} & - \text{C} & - \text{C} - \text{CH}_3 \\ & & & & & & \\ & \text{H} & \text{H} & & & \text{H} & \text{CH}_3 \end{array} $ <p>ALLOW any combination of skeletal OR structural OR displayed formula as long as unambiguous</p>
	Total	6	

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