OCR
Oxford Cambridge and RSA

GCE

Chemistry A

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

Advanced GCE

Mark Scheme for June 2017

H432A/02 **Mark Scheme**

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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.

Annotations available in RM Assessor

Annotation	Meaning
	Correct response
	Incorrect response
	Omission mark
BOD	Benefit of doubt given
CON	Contradiction
RE	Rounding error
SF	Error in number of significant figures
ECF	Error carried forward
L1	Level 1
L2	Level 2
L3	Level 3
NBOD	Benefit of doubt not given
SEEN	Noted but no credit given
I	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.

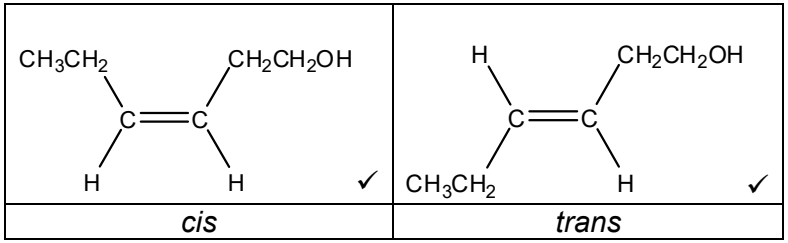
You should ensure that you have copies of these materials.

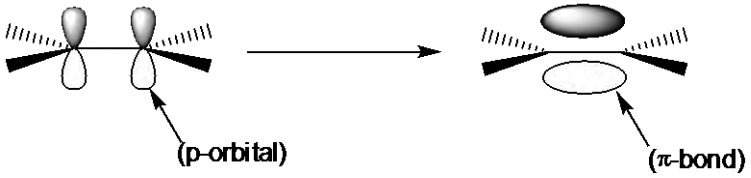
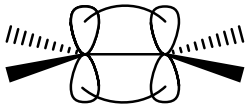
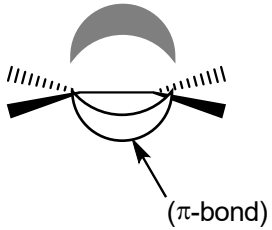
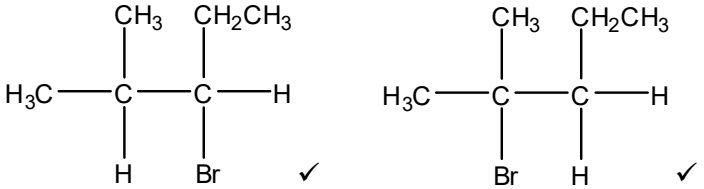
You should ensure also that you are familiar with the administrative procedures related to the marking process. These are set out in the OCR booklet **Instructions for Examiners**. If you are examining for the first time, please read carefully **Appendix 5 Introduction to Script Marking: Notes for New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

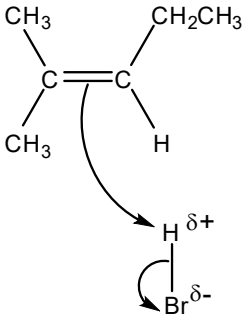
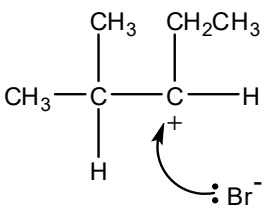
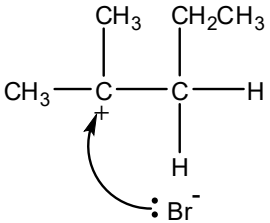
Please ask for help or guidance whenever you need it. Your first point of contact is your Team Leader.

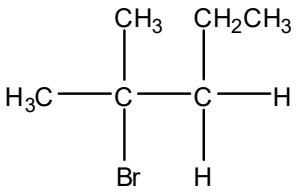
Question	Key	Marks	Guidance
1	B	1	
2	D	1	
3	C	1	
4	B	1	
5	D	1	
6	C	1	**ALLOW** 3 (This is the trigonal planar atom)
7	A	1	
8	C	1	**ALLOW** 4 (This is the number of chiral centres)
9	C	1	
10	D	1	
11	C	1	**ALLOW** 3 (This is the number of peaks in the NMR spectrum)
12	A	1	
13	A	1	
14	C	1	
15	A	1	

Question			Answer	Marks	Guidance
16	(a)		Compound **A** (is branched so) has less points of contact / less surface interaction between molecules ✓ Induced dipole–dipole interactions **/** London (dispersion) forces are weaker. **AND** Require less energy to break (these interactions / forces) ✓	**2**	**Both answers need to be comparisons** **ALLOW ORA** throughout **DO NOT ALLOW** 'more contact between atoms' **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) **ALLOW** fewer induced dipole-dipole interactions. **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.
	(b)	(i)	Hex-3-en-1-ol ✓	**1**	**ALLOW** Hex-3-ene-1-ol **ALLOW** 1-hydroxyhex-3-ene as this is unambiguous Hex-3-enol is **not** sufficient **IGNORE** lack of hyphens, or addition of commas

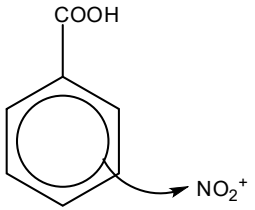
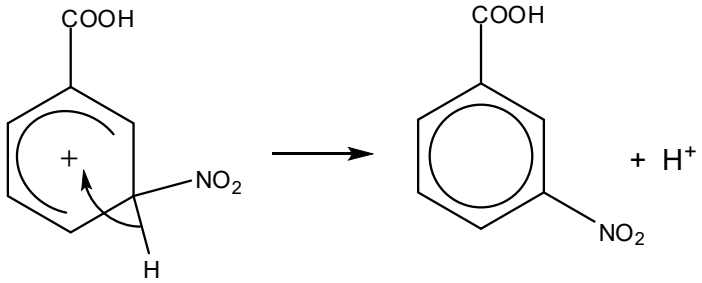
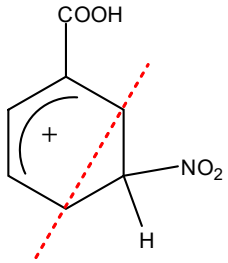
Question			Answer	Marks	Guidance
		(ii)	Same structural formula **AND** Different arrangement (of atoms) **in space OR** different **spatial** arrangement (of atoms) ✓	1	**ALLOW** have the same structure/displayed formula/skeletal formula **DO NOT ALLOW** same empirical formula **OR** same general formula **IGNORE** same molecular formula Reference to *E*/*Z* isomerism or optical isomerism is **not** sufficient
		(iii)	 *cis* ✓ *trans* ✓	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_2CH_2OH is represented as $-C_2H_5O$ or – C_2H_4OH **DO NOT ALLOW** incorrect connectivity e.g. – CH_3CH_2 on first occasion but allow **ECF** in second structure.

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

Question	Answer	Marks	Guidance
(iii)	Curly arrow from C=C bond to H of H–Br ✓ Correct dipole shown on H–Br **AND** curly arrow showing the breaking of H–Br bond ✓  --- Correct carbocation **AND** curly arrow from Br^- to C^+ of carbocation ✓  **OR**  	3	**ANNOTATE ANSWER WITH TICKS AND CROSSES** **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **DO NOT ALLOW** partial charges shown on C=C double bond (the second marking point) **DO NOT ALLOW** δ+ on C of carbocation 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)

Question			Answer	Marks	Guidance
		(iv)	 2-bromo-2-methylpentane **AND** (the) **carbocation** intermediate (in the formation of 2-bromo-2-methylpentane) is more stable (than the carbocation in the formation of the other product) ✓	1	**Note:** the correct product and explanation are **both** required for the mark The major product may be identified by its • corresponding letter (**E** or **F**) from the table in **(d)(ii)** • correct structure • correct name **DO NOT ALLOW** product comes from the more stable **secondary or primary** carbocation **IGNORE** explanations based on Markownikoff's rule.
	(e)	(i)	n(myrcene) = $\frac{204 \times 10^{-3}}{136.0}$ = 1.5(0) × 10^{-3} (mol) ✓ Volume of H_2 = 3 × 1.5(0) × 10^{-3} × 24000 = 108 (cm^3) ✓	2	Correct working **required** for the first marking point. **ALLOW ECF** from incorrect moles of myrcene i.e. n(myrcene) × 3 × 24000 **Common incorrect answers** 108000 cm^3 = 1 mark (not converted to g) 12cm^3 = 1 mark (divided by 3) 36 cm^3 = 1 mark (not multiplied by 3) **IGNORE** Calculations based on $pV = nRT$

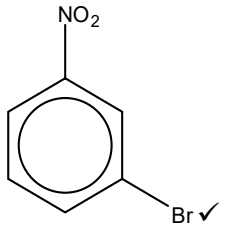
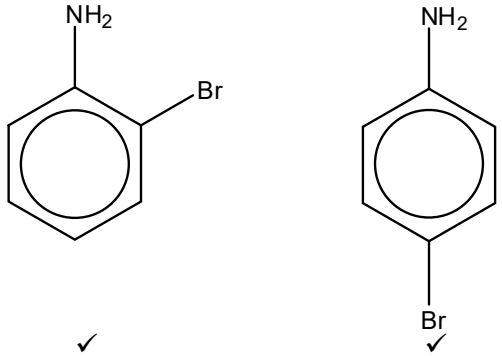
Question			Answer	Marks	Guidance
		(ii)	**Amount of hydrogen** $n(H_2) = \frac{5.28}{24.0} = 0.22(0)$ (mol) ✓ **Number of double bonds** $= \frac{0.220}{0.0200} = 11$ ✓ **Formula of saturated product** $C_{40}H_{78}$ ✓ **Equation** $C_{40}H_{56} + 11H_2 \longrightarrow C_{40}H_{78}$ ✓	**4**	**ALLOW**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

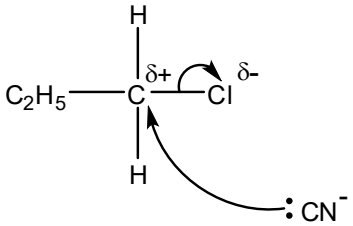
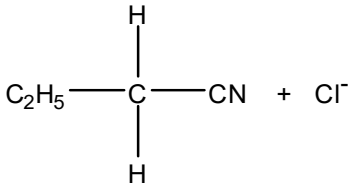
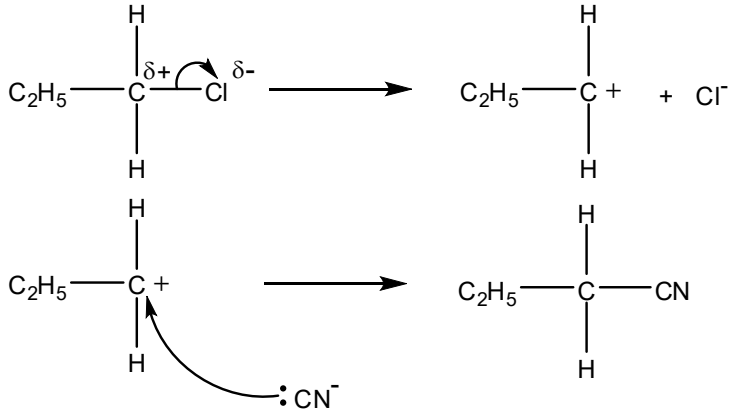
Question			Answer	Marks	Guidance
17	(a)	(i)	**Generation of electrophile** $HNO_3 + H_2SO_4 \longrightarrow H_2O + HSO_4^- + NO_2^+$ ✓ **Electrophilic substitution** Curly arrow from π-bond to NO_2^+ ✓  --- Correct intermediate ✓ Curly arrow back from C-H bond to reform π-ring **AND** H^+ as product ✓  **Regeneration of catalyst** $H^+ + HSO_4^- \longrightarrow H_2SO_4$ ✓	5	**ANNOTATE ANSWER WITH TICKS AND CROSSES** **ALLOW** $HNO_3 + 2H_2SO_4 \rightarrow H_3O^+ + 2HSO_4^- + NO_2^+$ **ALLOW** $HNO_3 + H_2SO_4 \rightarrow H_2NO_3^+ + HSO_4^-$ then $H_2NO_3^+ \rightarrow H_2O + NO_2^+$ **ALLOW** $^+NO_2$ **OR** NO_2^+ First curly arrow must come from the ring to NO_2^+ **DO NOT ALLOW** the following intermediate:  π-ring should cover approximately 4 of the 6 sides of the benzene ring structure **AND** the correct orientation, *i.e.* gap towards C with NO_2 **ALLOW** + sign anywhere inside the 'hexagon' of intermediate

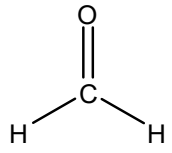
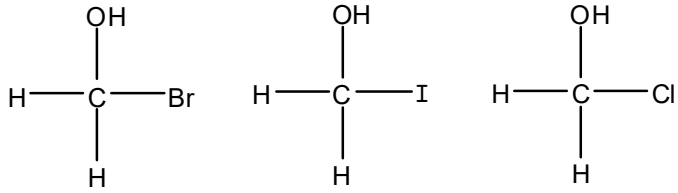
Question			Answer	Marks	Guidance
		(ii)*	*Please refer to the marking instructions on page 5 of this mark scheme for guidance on how to mark this question.* **Level 3 (5–6 marks)** Outlines the main steps of recrystallisation to produce a pure sample of 3-nitrobenzoic acid from the impure solid. **AND** Calculates correct percentage yield of 3-nitrobenzoic acid. **AND** Method of checking purity to include comparison to relevant data. *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.* **Level 2 (3–4 marks)** Attempts all three scientific points but explanations may be incomplete. **OR** Explains two scientific points thoroughly with very few omissions. *The description of checking for purity or recrystallisation is clear and any calculations structured. Key terminology used appropriately.* **Level 1 (1–2 marks)** A simple explanation based on at least two of the main scientific points. **OR**	6	**Indicative scientific points, with bulleted elements, may include:** **1. Purification** • Recrystallisation • Dissolve impure solid in minimum volume of hot water/solvent • Cool solution and filter solid • Wash with cold water/solvent and dry **2. Percentage yield** • n(benzoic acid) used = $\frac{4.97}{122}$ = 0.0407 (mol) • n(3-nitrobenzoic acid) made = $\frac{4.85}{167}$ = 0.0290 (mol) • percentage yield = $\frac{0.0290}{0.0407} \times 100$ = 71.3 (%) **ALLOW** 71 to calculator value of 71.29001554 correctly rounded. **CHECK** for extent of errors by **ECF** Alternative correct calculation may calculate theoretical mass of 3-nitrobenzoic acid that can be produced as 0.0407 × 167 = 6.80 (g) followed by: percentage yield = $\frac{4.85}{6.80} \times 100$ = 71.3 (%) Calculation **must** attempt to calculate n(benzoic acid) in mol. **3. Checking purity**

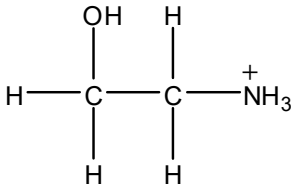
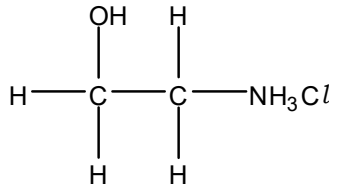
Question			Answer	Marks	Guidance
			Explains one scientific point thoroughly with few omissions. *There is an attempt at a logical structure. The description of the practical techniques provides some detail but may not be in the correct order.* • *Purification step is unclear with few scientific terms and little detail, e.g. just 'recrystallise'.* • *Calculation is difficult to follow, may just include a calculation of moles of reactants and/or products.* • *Purity check specifies a method but this is unclear with little detail, e.g. take melting point.* **0 marks** No response or no response worthy of credit.		• Obtain melting point • Compare to known values • Pure sample will have a (sharp) melting point very close to data book value **ALLOW** alternative approach based on spectroscopy or TLC **Spectroscopy** • Run an NMR/IR spectrum • Compare to (spectral) database • Spectrum of pure sample will contain same peaks and not others **TLC** • Run a TLC • Compare (R_f value) to known data • Pure sample will have a very similar R_f
	(b)	**(i)**	Phenol is the most easily nitrated/ most reactive **AND** Benzoic acid is the least easily nitrated /least reactive ✓	**1**	Response **must** give rank order of reactivity e.g. nitration becomes more difficult from phenol (to benzene) to benzoic acid **OR** nitration becomes easier from right to left in the table
		(ii)	**Reactivity of phenol** a (lone) pair of electrons on O is (partially) **delocalised/donated** into the π-system / ring ✓	**3**	**ANNOTATE ANSWER WITH TICKS AND CROSSES** **ALLOW** the electron pair in the p orbitals of the O atom becomes part of the π-system / ring **ALLOW** diagram to show movement of lone pair into ring

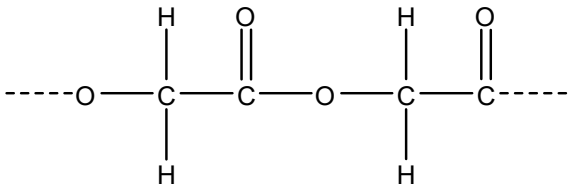
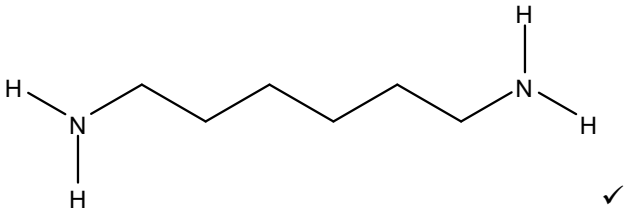
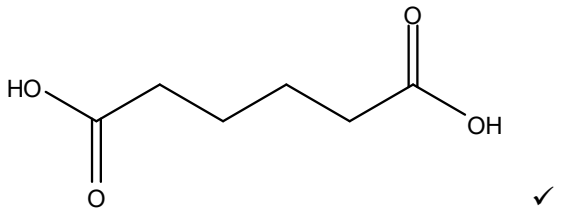
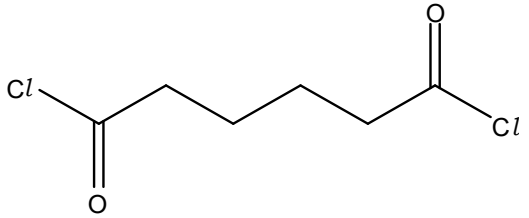
Question			Answer	Marks	Guidance
			Reactivity of benzoic acid The –COOH group on benzoic acid is an electron withdrawing group ✓ **Links electron density in π-bond to reactivity** In phenol electron density is higher **AND** The ring is more susceptible to attack **OR** In benzoic acid electron density is lower **AND** The ring is less susceptible to attack ✓		**ALLOW** lone pair of electrons on O is (partially) drawn/attracted/pulled into π-system / ring **IGNORE** activating and deactivating. **ALLOW** the following alternatives for susceptibility to attack: • 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)**	**Bromination**: Br_2 **AND** A*l*Br_3/$FeBr_3$/Fe ✓ **Intermediate**	**3**	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **ALLOW** any suitable halogen carrier catalyst

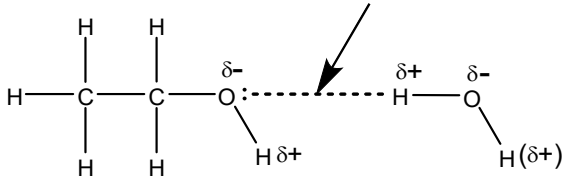
Question			Answer	Marks	Guidance
			 ✓ **Reduction**: Sn **AND** (concentrated) HC*l* ✓		**ALLOW** Kekulé structure **IGNORE** names *(question asks for formulae)* **IGNORE** reaction conditions even if incorrect **IGNORE** 'dilute' for HC*l* **IGNORE** H_2 **IGNORE** NaOH if seen as a reagent to convert nitro group into amine e.g 'Sn/(concentrated) HC*l* then NaOH' scores the mark
		(ii)	NH_2 is 2,4 directing ✓ Products (1 mark for each):  ✓ ✓	**3**	**IGNORE** references to electron donating/withdrawing groups **ALLOW** –NH_2 activates the ring causing the new group to join at positions 2 and 4. **ALLOW** ortho and para directing for 2,4 directing **IGNORE** 6-directing **ALLOW** Kekulé structure **IGNORE** names
			Total	**21**	

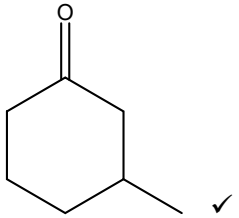
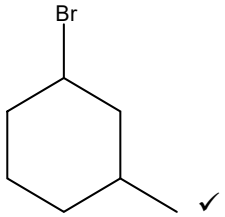
Question			Answer	Marks	Guidance
18	(a)	(i)	curly arrow from $^{-}$CN to carbon atom of C−C*l* bond ✓ Dipole shown on C–C*l* bond, $C^{\delta+}$ and $Cl^{\delta-}$, **AND** curly arrow from C−C*l* bond to C*l* atom ✓  --- correct organic product **AND** Cl^- ✓  	3	**ANNOTATE ANSWER WITH TICKS AND CROSSES** 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) **IGNORE** NaCl --- **ALLOW** S_N1 mechanism: Dipole shown on C–Cl bond, $C^{\delta+}$ and $Cl^{\delta-}$, **AND** curly arrow from C–C*l* bond to C*l* atom ✓ 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) ✓ correct organic product **AND** Cl^- ✓ 

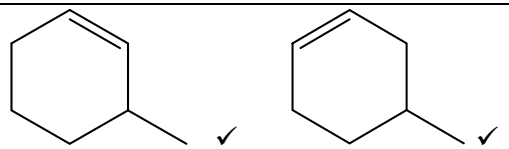
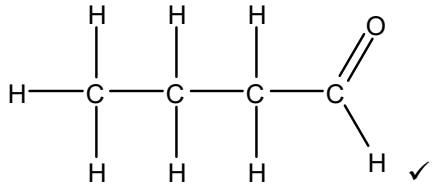
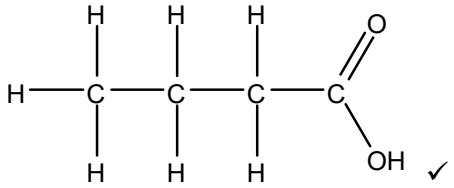
Question			Answer	Marks	Guidance
		(ii)	Compound **G**  ✓	3	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **IGNORE** name(s) **ALLOW** 
			Reagents **Reaction 2**: H_2 **AND** Ni ✓		**ALLOW** any suitable metal catalyst e.g. Pt **ALLOW** $LiAlH_4$ for reagent in reaction 2 **DO NOT ALLOW** $NaBH_4$ for reagent in reaction 2 **IGNORE** names *(question asks for formulae)* **IGNORE** references to temperature and/or pressure
			Reaction 3: Correct formula of an **aqueous** acid e.g. HC*l*(aq)/H_2SO_4(aq) ✓		**ALLOW** H^+(aq) **IGNORE** dilute **ALLOW** formula of an acid **AND** water e.g. HC*l* **AND** H_2O H_2SO_4 **AND** H_2O

Question			Answer	Marks	Guidance
		(iii)	**Explanation** Nitrogen electron pair **OR** nitrogen lone pair **AND** accepts a proton/H^+ ✓ **Structure of salt**  **AND** Cl^- ✓	**2**	**IGNORE** NH_2 group donates electron pair **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 Compound **H** is a base is **not** sufficient *(role of lone pair required)* **DO NOT ALLOW** nitrogen/N lone pair accepts hydrogen (*proton/H^+ required)* **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **ALLOW**  *i.e.* charges **not** required **IF** charges are shown **both** need to be present **ALLOW** charge either on N atom or NH_3^+ **IF** displayed then + charge must be on the nitrogen

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

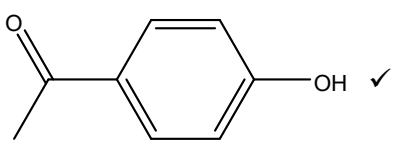
Question			Answer	Marks	Guidance
19	(a)		$C_5H_{10}O + 7O_2 \longrightarrow 5CO_2 + 5H_2O$ ✓	1	**ALLOW** multiples e.g. $2C_5H_{10}O + 14O_2 \longrightarrow 10CO_2 + 10H_2O$ **ALLOW** any equation involving an unsaturated alcohol with correct balancing **e.g.** $C_5H_8O + 6.5O_2 \longrightarrow 5CO_2 + 4H_2O$ $C_5H_6O + 6O_2 \longrightarrow 5CO_2 + 3H_2O$ $C_5H_4O + 5.5O_2 \longrightarrow 5CO_2 + 2H_2O$ $C_5H_2O + 5O_2 \longrightarrow 5CO_2 + H_2O$ **IGNORE** state symbols
	(b)	(i)	Diagram showing a water molecule and an ethanol molecule with at least one $H^{\delta+}$ and one $O^{\delta-}$ on **BOTH** molecules ✓ Hydrogen bond between one lone pair on O atom in one of the molecules and the H atom of another. **AND** Hydrogen bonding stated or labelled on diagram ✓ e.g. Hydrogen bond  	2	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **DO NOT ALLOW** δ+ on H atoms of alkyl group **DO NOT ALLOW** any marks for a diagram containing O_2H If more than one hydrogen bond is shown they must **all** be correct to award the mark.

Question			Answer	Marks	Guidance
		(ii)	Hexane-1,6-diol has more OH groups (than hexan-1-ol) **AND** (hexane-1,6-diol) forms more hydrogen bonds **with water** ✓	1	Statements **MUST** be comparative e.g. hexane-1,6-diol has two –OH groups and hexan-1-ol has one -OH group **ALLOW** hydroxyl or hydroxy **DO NOT ALLOW** hydrox**ide**/OH^- **ALLOW ORA**
	(c)	(i)	**Starting material from reduction reaction**  ✓ **Reagent for reduction** $NaBH_4$ ✓ **Product from reaction with $NaBr/H_2SO_4$**  ✓ **Structural isomers**	5	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous Watch for missing methyl groups **IGNORE** H^+ / acid or H_2O or ethanol **ALLOW** sodium borohydride **OR** sodium tetrahydridoborate **ALLOW** $LiAlH_4$

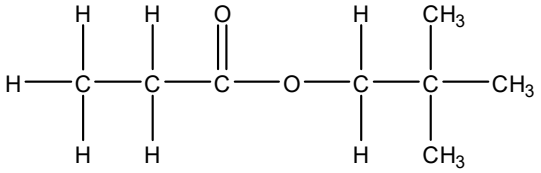
Question			Answer	Marks	Guidance
			 ✓ ✓		**ALLOW** in either order
		(ii)	3-methylcyclohexanol ✓	**1**	**ALLOW** 3-methylcyclohexan-1-ol **ALLOW** 1-methylcyclohexan-3-ol **IGNORE** lack of hyphens, or addition of commas
	(d)		**Structures of organic products**  ✓  ✓ **Equations** $CH_3CH_2CH_2CH_2OH + [O] \longrightarrow CH_3CH_2CH_2CHO + H_2O$ ✓ $CH_3CH_2CH_2CH_2OH + 2[O] \longrightarrow CH_3CH_2CH_2COOH + H_2O$ ✓ **Reaction conditions**	**5**	**ANNOTATE WITH TICKS AND CROSSES** Use of any primary alcohol containing 3, 5 or more carbons can be awarded up to 4 marks. **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **IGNORE** names **DO NOT ALLOW** $CH_3CH_2CH_2COH$ for the structure of the aldehyde. **ALLOW** $CH_3CH_2CH_2CO_2H$ for the structure of the carboxylic acid. **ALLOW** marks for structures from equations as long as unambiguous. **ALLOW** molecular formulae in equations e.g. $C_4H_{10}O + [O] \longrightarrow C_4H_8O + H_2O$ $C_4H_{10}O + 2[O] \longrightarrow C_4H_8O_2 + H_2O$ $C_4H_9OH + [O] \longrightarrow C_3H_7CHO + H_2O$ $C_4H_9OH + 2[O] \longrightarrow C_3H_7CO_2H + H_2O$ **IGNORE** incorrect structures in equations i.e. $C_4H_{10}O + [O] \longrightarrow C_3H_7COH + H_2O$

Question			Answer	Marks	Guidance
			Distillation to produce aldehyde/$CH_3CH_2CH_2CHO$ **AND** Reflux to produce carboxylic acid/$CH_3CH_2CH_2COOH$ ✓		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 = C_4H_4O ✓ **Molecular formula** Molecular formula = $C_8H_8O_2$ **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_2CO_3 (so not carboxylic acid) ✓ Links 2,4-DNP(H) or Brady's reagent observation to carbonyl **AND** Tollens' reagent observation (so not an aldehyde) ✓		**ALLOW** identity of functional groups in the explanation if not stated on functional group prompt line. **ALLOW** "aldehyde or ketone" in place of carbonyl
	(c)		**Carbon NMR analysis** Peaks between 110–160 ppm are the (four) aromatic (carbon environments) ✓ Compound contains a C=O between 190 - 200 ppm **AND** Compound contains a C-C at 20-30 ppm ✓ **Structure**  ✓	**3**	**ALLOW** peaks to be identified by: • Peaks labelled on spectrum • Peaks indicated on a chemical structure • Peaks indicated from within text **Note:** If identifying aromatic peaks from the spectrum all four peaks should be indicated. **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous
			Total	**9**	

Question	Answer	Marks	Guidance
21*	*Please refer to the marking instructions on page 5 of this mark scheme for guidance on how to mark this question.* **Level 3 (5–6 marks)** Structure of **L** is $CH_3CH_2COOCH_2C(CH_3)_3$ **OR** $(CH_3)_3CCH_2COOCH_2CH_3$ **AND** A comprehensive explanation with **most** of the spectral data analysed and few omissions. *There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.* *Splitting patterns used to deduce the correct structure of **L**.* **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. *There is a line of reasoning presented with some structure. The information presented in the most part relevant and supported by some evidence.* *The analysis is clear and includes some interpretation of NMR/IR peaks.* **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. *There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.*	6	**Indicative scientific points may include:** **1. ^{1}H NMR spectrum** • δ = 1.1 ppm, triplet, 3H **CH_3**–CH_2– • δ = 1.3 ppm, singlet, 9H **$(CH_3)_3$**C– • δ = 2.3 ppm, quartet, 2H CH_3–**CH_2**–C=O • δ = 4.0 ppm, singlet, 2H –**CH_2**–O– **ALLOW** approximate values for chemical shifts. **2. Infrared spectra** IR spectrum of **M** • peak at 2300–3700 (cm^{-1}) is O–H • peak at ~1720 (cm^{-1}) is C=O • **M** is a carboxylic acid IR spectrum of **N** • peak at 3100-3700 (cm^{-1}) is O–H • **N** is an alcohol **ALLOW** ranges from *Data Sheet* **IGNORE** references to C–O peaks **3. Structure of L** • **L** is an ester (as it reacts with HC*l*(aq) to form carboxylic acid and alcohol)

Question			Answer	Marks	Guidance
			The analysis is communicated in an unstructured way and includes interpretation of a few peaks from the NMR/IR spectra. **0 marks** No response or no response worthy of credit.		• Correct structure  **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous
			Total	**6**	

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