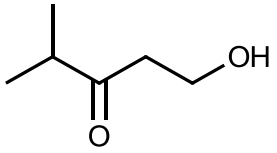
Mark Scheme

Question	Key	Marks	Guidance
1	A	**1**	

Mark Scheme

Question	Answer	Marks	Guidance
2	*Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question.* **Level 3 (5–6 marks)** Structure correct **AND** Analysed all ^{1}H NMR signals with at least two supporting statements made. *The analysis is clear and logically structured. The supporting statements are relevant to the correct structure drawn.* **Level 2 (3–4 marks)** Structure has correct molecular formula **AND** C=O **AND** OH but in incorrect positions **AND** Analysed at least three ^{1}H NMR signals with one or two supporting statements made *The analysis is presented with some structure. The supporting statements are in the most-part relevant to the structure drawn.* **Level 1 (1–2 marks)** Structure has correct molecular formula **AND** C=O **OR** OH but in incorrect positions **AND** Analysed at least two ^{1}H NMR signals with no or one supporting statements made *The analysis is basic and communicated in an unstructured way. The relationship of the supporting evidence to the structure may not be clear.*	**6**	**Indicative scientific points may be included:** **Structure**  **L** = **^{1}H NMR spectrum** δ = 3.8 ppm, triplet, 2H CH_2—**CH_2—O** δ = 3.7 ppm, singlet, 1H O—**H** δ = 3.1 ppm, triplet, 2H CH_2—**CH_2C=O** δ = 2.7 ppm, septet, 1H $(CH_3)_2$C**HC=O** δ = 1.0 ppm, doublet, 6H **$(CH_3)_2$**CH **Supporting statements** δ = 3.7 ppm lost after D_2O, indicating —O**H** δ = 213 ppm in ^{13}C NMR but no δ = 9–10 ppm in ^{1}H NMR so ketone, **not** aldehyde $M_r(C_3H_6O)$ = 58 116/58 = 2 → $C_6H_{12}O_2$

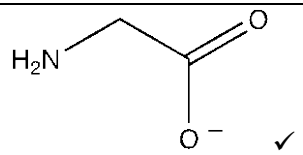
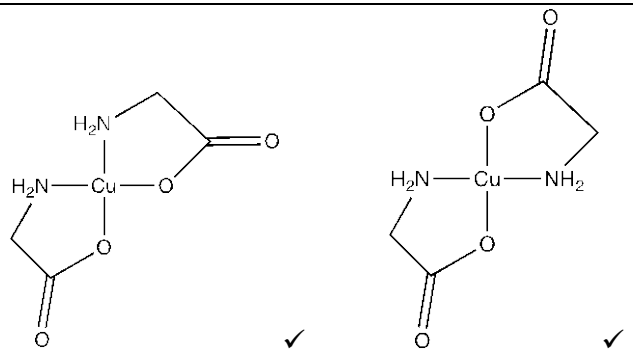
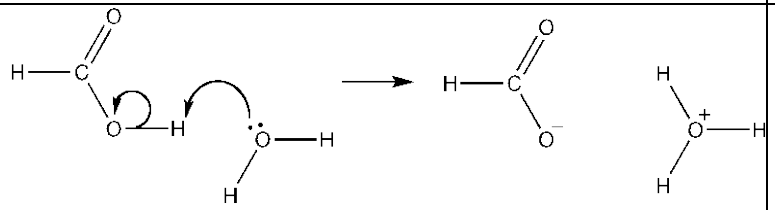
Mark Scheme

Question			Answer	Marks	Guidance
			0 marks No response or no response worthy of credit.		
			Total	**6**	

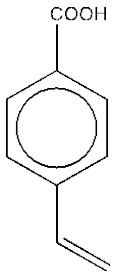
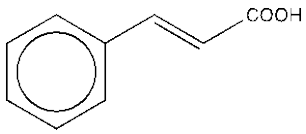
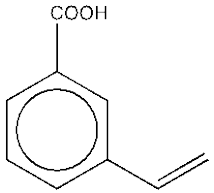
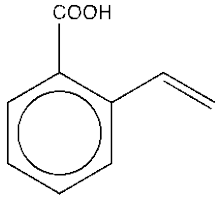
Mark Scheme

Question			Answer	Marks	Guidance
3	(a)	(i)	reaction with bases: neutralisation **AND** reaction with metals: redox ✓	1	
		(ii)	correctly calculates n(**A**) = $\frac{1.125}{90}$ = 0.0125 (mol) ✓ volume of H_2 = $\frac{0.0125}{2}$ x 24,000 = 150 cm^3 ✓ **units** required	2	**ALLOW** 0.15 dm^3 **ALLOW ECF** from n(**A**)
		(iii)	$C_6H_{12}O_6Mg$ ✓	1	**DO NOT ALLOW** $(C_3H_6O_3)_2Mg$
		(iv)	Type of reaction of COOH: e.g. esterification **AND** reagents and conditions e.g. CH_3OH **AND** H_2SO_4 ✓ Organic product of COOH reaction ✓ Type of reaction of –OH **AND** reagents and conditions ✓ Organic product of –OH reaction ✓	4	**ALLOW** esterification with any stated alcohol e.g. product from CH_3OH/H_2SO_4 → $CH_3(CHOH)COOCH_3$ Many possible reactions of secondary alcohol possible, e.g. oxidation with $K_2Cr_2O_7/H_2SO_4$ + heat → $CH_3(CO)COOH$ elimination with H_2SO_4/H_3PO_4 + heat → CH_2=$CHCOOH$ esterification with CH_3COOH/H_2SO_4 **OR** CH_3COCl → $CH_3(CHOOCCH_3)COOH$ bromination with $NaBr/H_2SO_4$ → $CH_3(CHBr)COOH$ **ALLOW** self-polymerisation as reaction for either

Mark Scheme

Question			Answer	Marks	Guidance
					group (if another reaction example given) condensation polymerisation with H_2SO_4 $\rightarrow [OCH(CH_3)CO]_n$
	(b)	**(i)**	 ✓	**1**	Must be skeletal formula
		(ii)	 ✓ ✓	**2**	**IGNORE** charges **ALLOW** Cs and Hs labelled on structures *Marks are for correct connectivity*
		(iii)	Alanine has a chiral C atom/centre ✓	**1**	
	(c)		 1 mark for correct reactants **AND** products **AND** correct positioning of + and – charges on products ✓ 1 mark for two correct curly arrows **AND** H_2O curly arrow starting from O lone pair ✓	**2**	

Mark Scheme

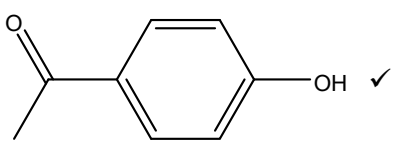
Question			Answer	Marks	Guidance
	(d)		Electrophilic substitution means benzene ring ✓ Electrophilic addition means alkene / C=C ✓ Isomer of $C_9H_8O_2$ containing C=C, benzene ring **AND** COOH ✓ Correct isomer:  **OR**  ✓ justification in terms of number of carbon environments ✓	**5**	Concluded using data provided and conclusions from 1st two marks. **ALLOW** 1 mark for:  **OR**  (does not gain final justification mark)
			Total	**19**	

Mark Scheme

Question	Key	Marks	Guidance
4	C	1	**ALLOW** 3 (This is the number of peaks in the NMR spectrum)

Question			Answer	Marks	Guidance
5	(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.

Mark Scheme

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**	

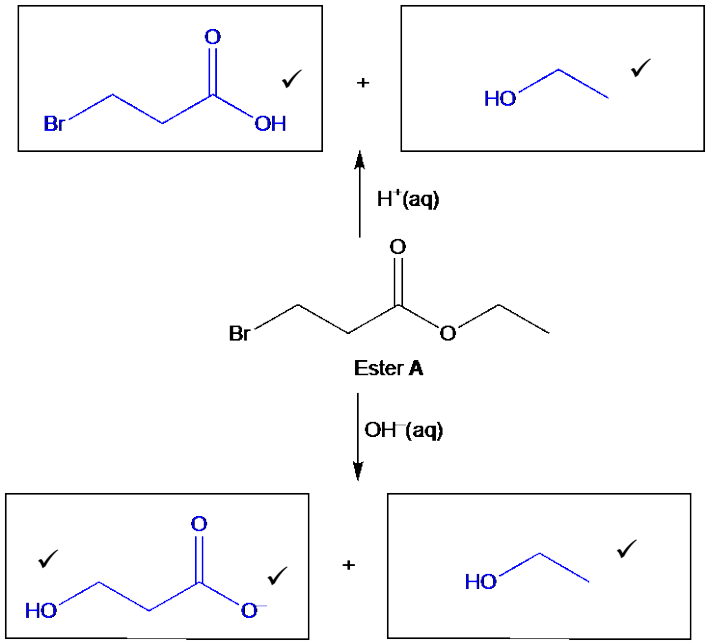
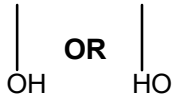
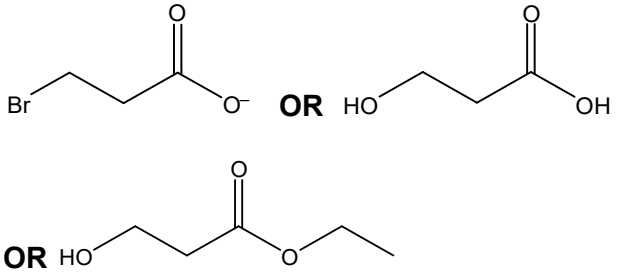
Mark Scheme

Question	Answer	Marks	Guidance
6	A	1	
7	B	1	**ALLOW** 4 (This is the number of peaks in the NMR spectrum)

Mark Scheme

Question	Answer	Marks	AO element	Guidance
8	**B**	**1**	AO2.5	
9	**C**	**1**	AO2.5	

Mark Scheme

Question			Answer	Marks	AO element	Guidance
10	(a)	(i)	ethyl 3-bromopropanoate ✓	1	AO1.2	**ALLOW** one word: ethyl3-bromopropanoate **OR** more words, e.g. ethyl 3-bromo propanoate **IGNORE** lack of hyphens, or addition of commas
		(ii)		5	AO2.5 ×5	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **ALLOW** in either order **ALLOW** any vertical bond to the OH group e.g. **ALLOW**  **DO NOT ALLOW** OH– **ALLOW** in either order For reaction with OH^-, **ALLOW** one mark for 

Mark Scheme

<table>
<tr><th colspan="3">Question</th><th>Answer</th><th>Marks</th><th>AO element</th><th>Guidance</th></tr>
<tr><td></td><td></td><td>(iii)</td><td>hydrolysis ✓</td><td>1</td><td>AO1.1</td><td>IGNORE ‘acid’ and ‘alkaline’’
IGNORE nucleophilic substitution</td></tr>
<tr><td></td><td>(b)</td><td></td><td>
<table>
<tr><th>Proton environment</th><th>Chemical shift</th><th>Splitting pattern</th></tr>
<tr><td>1</td><td>3.0–4.3</td><td>Triplet</td></tr>
<tr><td>2</td><td>2.0–3.0</td><td>Triplet</td></tr>
<tr><td>3</td><td>3.0–4.3</td><td>Quartet</td></tr>
<tr><td>4</td><td>0.5–1.9</td><td>Triplet</td></tr>
</table>
Mark by column
Chemical shift: all 4 correct ✓✓
3 correct ✓

Splitting pattern: all 4 correct ✓✓
3 correct ✓</td><td>4</td><td>AO3.1
× 4</td><td>ALLOW δ values ± 0.2 ppm, as a range or a value within the range

ALLOW integers for δ values
e.g. 2 is equivalent to 2.0

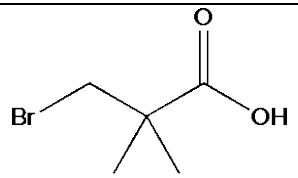
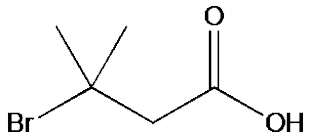
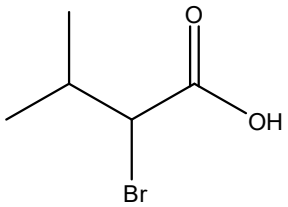
ALLOW quadruplet for quartet

ALLOW diagrams to show splitting pattern
e.g.
  for triplet

  for quartet

ALLOW splitting patterns shown as numbers
i.e. ‘3’ for triplet, ‘4’ for quartet</td></tr>
</table>

Mark Scheme

Question			Answer	Marks	AO element	Guidance
	(c)		 **OR**  **OR**  ✓	**1**	AO3.1	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous
	(d)		**IF** answer on answer line = 24018, **AWARD** 2 marks **IF** answer on answer line = 27600, **AWARD** 1 mark --- Relative mass of 200 molecules = 200 × 138 = 27600 ✓ M_r of polyester = 27600 – 199 × 18 = 24018 ✓	**2**	AO2.2 ×2	**ALLOW ECF** from incorrect M_r Alternative method based on repeat unit: M_r of 200 repeat units = 200 x 120 = 24000 ✓ M_r of polymer = 24000 + 1 + 17 = 24018 ✓
	(e)	(i)*	*Refer to marking instructions on page 4 of mark scheme*	**6**	AO3.3	**Indicative scientific points may include:**

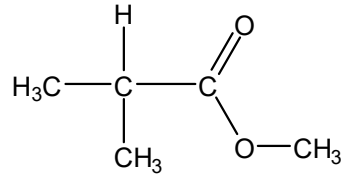
Mark Scheme

Question	Answer	Marks	AO element	Guidance
	for guidance on marking this question. **Level 3 (5-6 marks**) Correct calculation of the mass of $(CH_3)_2CHCHO$. **AND** Planned synthesis includes oxidation of aldehyde and formation of ester **C** with most of the reagents and conditions identified and equations are mostly correct. *There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.* **Level 2 (3-4 marks)** Calculation of the mass of $(CH_3)_2CHCHO$ is partly correct **AND** Planned synthesis includes oxidation of aldehyde and formation of ester **C** with some of the reagents and conditions identified **OR** Attempts to calculate mass of $(CH_3)_2CHCHO$ but makes little progress **AND** Planned synthesis includes oxidation of aldehyde and formation of ester **C** with most of the reagents and conditions identified and equations for each step are mostly correct *There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.*		×6	**<u>Calculation of mass of $(CH_3)_2CHCHO$</u>** **Using moles** • $n(\text{ester}) = \frac{12.75}{102.0}$ = 0.125 (mol) • $n((CH_3)_2CHCHO) = 0.125 \times \frac{100}{40}$ = 0.3125 (mol) • Mass of $(CH_3)_2CHCHO = 72.0 \times 0.3125$ = 22.5 g **Using mass** • Theoretical mass of ester = $12.75 \times \frac{100}{40}$ = 31.875 (g) • Theoretical $n((CH_3)_2CHCHO) = \frac{31.875}{102}$ = 0.3125 (mol) • Mass of $(CH_3)_2CHCHO = 72.0 \times 0.3125$ = 22.5 g **ALLOW** small slip/rounding errors such as errors in *Mr* e.g. use of 71 instead of 72 for $(CH_3)_2CHCHO$ **----------** ***Examples of partly correct calculations*** Mass = 3.60 g from $0.125 \times \frac{40}{100} \times 72$ (*% yield inverted*) Mass = 9.00 g from 0.125×72 (*% yield omitted*)

Mark Scheme

Question			Answer	Marks	AO element	Guidance
			Level 1 (1-2 marks) Calculation of the mass of $(CH_3)_2CHCHO$ is partly correct **OR** Planned synthesis includes both steps with some of the reagents and conditions identified **OR** Attempts equations for both steps but these may contain errors **OR** Describes one step of the synthesis with reagents, conditions and equation mostly correct *There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.* **0 marks** No response or no response worthy of credit.			**<u>Synthesis: reagents and conditions</u>** ***Step 1:*** Oxidation of aldehyde $(CH_3)_2CHCHO$ • Reagents: $Cr_2O_7^{2-}/H^+$ • Conditions: reflux • Equation: $(CH_3)_2CHCHO + [O] \rightarrow (CH_3)_2CHCOOH$ ***Step 2:*** Formation of ester C • Reagents**:** methylpropanoic acid/$(CH_3)_2CHCOOH$ and methanol/CH_3OH • Conditions: acid (catalyst) reflux/heat • Equation: $(CH_3)_2CHCOOH + CH_3OH \rightarrow (CH_3)_2CHCOOCH_3 + H_2O$ **IGNORE** attempts to form methanol in synthesis
	(e)	**(ii)**		**2**	AO2.7 × 2	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous

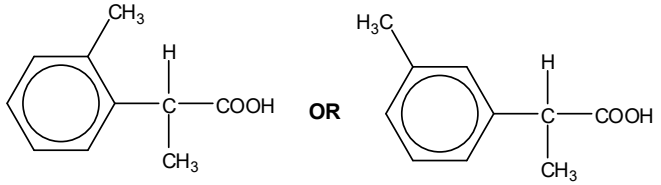
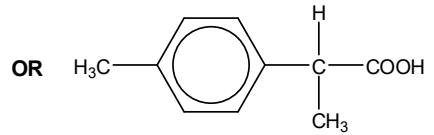
Mark Scheme

Question			Answer	Marks	AO element	Guidance
			Y (43) = $(CH_3)_2CH^+$ ✓ **Z** (71) $(CH_3)_2CHCO^+$ ✓ *If '+' charge is missing/incorrect but the structures of **both** fragments are correct, award one mark*			**ALLOW** positive charge to be anywhere on the structure For **Y** and **Z**, **ALLOW** structure of a feasible fragment ion formed from ester **C**  **Ester C** e.g. **Y** (43) = CH_3OC^+ **Z** (71) = $^+CCOOCH_3$ **ALLOW** 1 mark if both correct **ions** are shown but in the incorrect columns **ALLOW** 1 mark for both correct **ions** if one or both have an 'end bond' **ALLOW** 1 mark if both **ions** are shown using correct molecular formulae
			Total	**22**		

Mark Scheme

Question	Answer	Marks	AO element	Guidance
11	*Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question.* **Level 3 (5–6 marks)** Structure is $CH_3C_6H_4CH(CH_3)COOH$ **AND** Most of the data analysed. *There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.* **Level 2 (3–4 marks)** A viable aromatic structure of $C_{10}H_{12}O_2$ that contains C=O **AND** most key features consistent with spectral data **AND** Some of the spectral data analysed *There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.*	**6**	AO1.2 × 2 AO3.1 × 2 AO3.2 × 2	**Indicative scientific points:** **<u>Empirical and Molecular Formulae</u>** • C : H : O = $\frac{73.17}{12.0} : \frac{7.32}{1.0} : \frac{19.51}{16.0}$ = 6.10 : 7.32 : 1.22 = 5 : 6 : 1 • Empirical formula = C_5H_6O • uses *m/z* = 164.0 to determine molecular formula as $C_{10}H_{12}O_2$ **<u>Structure</u>** **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **Key features of an aromatic structure consistent with spectral data** • COOH group • 4 aromatic H atoms • single H atom that would give a quartet • CH_3 group that would give a doublet • CH_3 group that would give a singlet

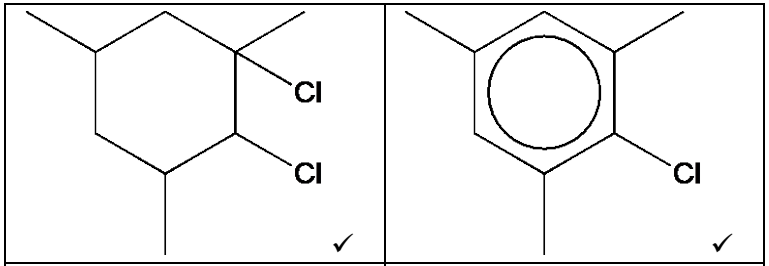
Mark Scheme

Question	Answer	Marks	AO element	Guidance
	Level 1 (1–2 marks) Correct determination of empirical formula and/or molecular formula. **OR** Analyses some of the IR and NMR data. **OR** Analyses most of the NMR data. *There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.* **0 marks** No response or no response worthy of credit.			**Correct Structure** • $CH_3C_6H_4CH(CH_3)COOH$ **ALLOW** 2-, 3- **OR** 4- substitution of ring *i.e.*   **<u>Spectral analysis</u>** **^{1}H NMR** • δ = 1.6 ppm, doublet, 3H **CH_3**–CH– • δ = 2.3 ppm, singlet, 3H Ar-C**H_3** • δ = 2.7 ppm, quartet, 1H CO–**CH**–CH_3 **OR** Ar–**CH**–CH_3 / C_6H_5–**CH**–CH_3 • δ = 7.1–7.5 ppm, multiplet, 4H C_6**H_4**– **ALLOW** approximate values for chemical shifts. **IR:** • peak at 2300–3700 (cm^{-1}) is O–H • peak at ~1720 (cm^{-1}) is C=O • unknown is a carboxylic acid **ALLOW** ranges from *Data Sheet* **IGNORE** references to C–O peaks
	Total	**6**		

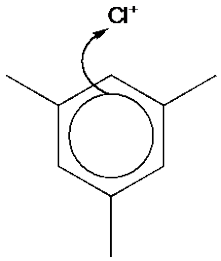
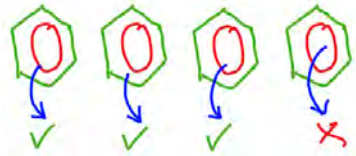
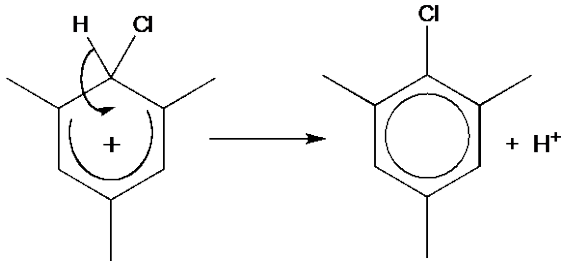
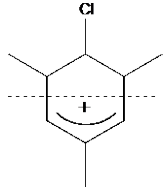
Mark Scheme

Question	Answer	Marks	AO element	Guidance
12	C	1	2.2	

Mark Scheme

Question			Answer	Marks	AO element	Guidance
13	(a)	(i)	 ✓ Organic product with **B** ✓ Organic product with **C**	**2**	**2.5×2**	
		(ii)	**Reactivity of B** in B electrons are localised OR in B π-bond is localised ✓ **Reactivity of C** in C electrons are delocalised OR In C π-system / ring is delocalised In **B**, electron density is higher **AND** B is more susceptible to electrophilic attack **OR** B attracts/accepts the electrophile/Cl_2 more **OR** B polarises the electrophile/Cl_2 more ✓ **ORA**	**3**	**1.1×3**	**ALLOW** labelled diagram to show delocalised system **IGNORE** charge density **IGNORE** electronegativity **IGNORE** B is more reactive/reacts more readily (no reference to electrophile) **IGNORE** references to electron density spread around the π–ring **ALLOW** chlorine

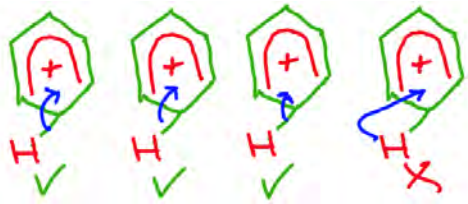
Mark Scheme

Question	Answer	Marks	AO element	Guidance
(iii)	**Generation of electrophile** $AlCl_3 + Cl_2 \rightarrow AlCl_4^- + Cl^+$ ✓	5	1.2	**ANNOTATE ANSWER WITH TICKS AND CROSSES** **ALLOW** $FeCl_3 + Cl_2 \rightarrow FeCl_4^- + Cl^+$ **ALLOW** use of Fe
	Attack of Cl^+  Curly arrow from π-bond to Cl^+ ✓		1.2	**NOTE**: curly arrows can be straight, snake-like, etc. …….. but **NOT** double-headed or half-headed arrows **1st curly arrow** must • start from, **OR** close to, **circle of benzene ring** 
	---------- **Intermediate and organic product**  Correct intermediate ✓		2.5	**DO NOT ALLOW** following intermediate: 
	Curly arrow from C–H bond to reform π-ring ✓		1.2	π-ring must cover 4 of the 6 sides of the benzene ring **AND** correct orientation, *i.e.* gap towards C–Cl
	---------- **Regeneration of catalyst** $H^+ + AlCl_4^- \rightarrow AlCl_3 + HCl$ ✓		1.2	**ALLOW** + sign anywhere inside the 'hexagon' of the intermediate.

Mark Scheme

<table>
<tr><th colspan="3">Question</th><th>Answer</th><th>Marks</th><th>AO element</th><th>Guidance</th></tr>
<tr><td></td><td></td><td></td><td></td><td></td><td></td><td>IGNORE partial charges on the chlorine in the intermediate

DO NOT ALLOW mark for intermediate if any CH_3 is missing

Curly arrow must start from, OR be traced back to, any part of C-H bond and go inside the ‘hexagon’
 

ALLOW use of $AlCl_4^-$ in the mechanism

ALLOW ECF for regeneration of an incorrect metal chloride catalyst e.g. $AgCl_3$</td></tr>
<tr><td></td><td>(b)</td><td></td><td>$3C_3H_6O \rightarrow C_9H_{12} + 3H_2O$

molecular formulae of C_3H_6O AND C_9H_{12} ✓

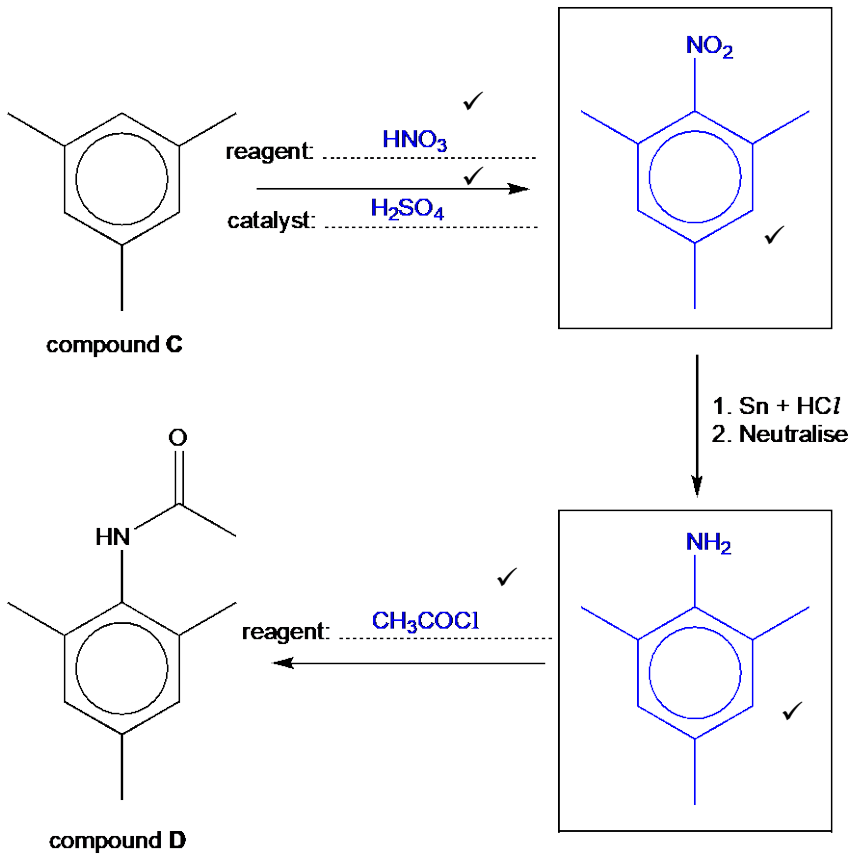
H_2O as by-product ✓

correct balanced equation ✓</td><td>3</td><td>2.6

2.5

2.6</td><td></td></tr>
<tr><td></td><td>(c)</td><td>(i)</td><td><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></td><td>2</td><td>3.2</td><td></td></tr>
</table>

Mark Scheme

Question	Answer	Marks	AO element	Guidance
(ii)		5	3.2×5	**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous **IGNORE** names for organic intermediates (question asks for structures **ALLOW** names of reagents and catalyst Around top arrow, **ALLOW** 1 of 2 marks if HNO_3 and H_2SO_4 swapped. i.e. reagent: H_2SO_4 catalyst: HNO_3 **IGNORE** references to concentration **ALLOW** $(CH_3CO)_2O$ for left arrow **IGNORE** CH_3COOH **IGNORE** acyl chloride **DO NOT ALLOW** $AlCl_3/FeCl_3$/Fe4

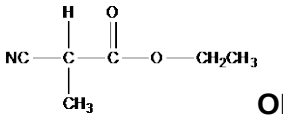
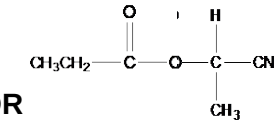
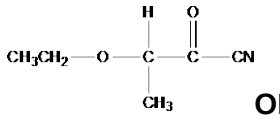
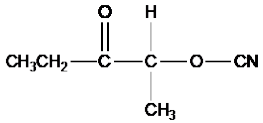
Mark Scheme

Question			Answer	Marks	AO element	Guidance
14	(a)*		*Refer to marking instructions on page 4 of mark scheme for guidance on marking this question.* **Level 3 (5-6 marks**) A correct calculation of the mass of cyclopentanol **AND** A **detailed** description of most purification steps *There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.* **Level 2 (3-4 marks)** Calculates the mass of cyclopentanol with some errors **AND** A **detailed** description of some purification steps **OR** A correct calculation of the mass of cyclopentanol **AND** A **detailed** description of a few purification steps *There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.* **Level 1 (1-2 marks)** Calculates the mass of cyclopentanol with some errors **OR** A **detailed** description of some purification steps *There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.* **0 marks** No response or no response worthy of credit.	**6**	**2.8×2** **3.3×4**	**Indicative scientific points may include:** **<u>Calculation of mass of cyclopentanol</u>** **Using moles** • n(cyclopentene) = $\frac{4.00}{68}$ = 0.0588…. (mol) • n(cyclopentanol) = 0.0588 × $\frac{100}{64}$ = 0.0919…(mol) • Mass of cyclopentanol = 86 × 0.0919 = **7.90** g **Using mass** • Theoretical mass cyclopentene= 4.00 × $\frac{100}{64}$ = 6.25 g • Theoretical n(cyclopentanol) = $\frac{6.25}{68}$ = 0.0919 (mol) • Mass of cyclopentanol = 86 × 0.0919 = **7.90** g **ALLOW** for small slip in Mr / rounding errors **<u>Examples of some calculation errors</u>** **Incorrect inverse ratio**: • 0.0588 × $\frac{64}{100}$ = 0.0376…. (mol) • Mass = 86 × 0.0376 = 3.24 g **Ignoring % yield gives**: • $\frac{4.00}{68}$ = 0.0588…. (mol) • Mass = 86 × 0.0588 = 5.06 g **<u>Purification</u>** • Add a neutralising agent **by formula or name** e.g. Na_2CO_3 • In separating funnel, **organic layer is on top** • Drying with an **anhydrous salt by formula or name**, e.g. $MgSO_4$, Na_2SO_4, $CaCl_2$ • Redistil **at approx. 44ºC** **Examples** of detail in **bold** (**NOT INCLUSIVE**)

Mark Scheme

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

Mark Scheme

Question		Answer	Marks	AO element	Guidance
15	**(a)**	$CDCl_3$ used as a solvent ✓ D_2O used to identify OH **OR** NH protons ✓	**2**	**1.1×2**	Example and use required for each mark **ALLOW** for 1 mark, D_2O as a solvent
	(b)*	*Please refer to the marking instructions on page 4 of this mark scheme for guidance on how to mark this question.* **Level 3 (5–6 marks)** Structure **I** has a viable chemical structure of $C_6H_9NO_2$ which has the key features consistent with spectral data **AND** Most of the data analysed *There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.* **Level 2 (3–4 marks)** Compound **I** has a viable chemical structure of $C_6H_9NO_2$ with most of the key features consistent with spectral data **AND** Some of the spectral data analysed. *There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.* **Level 1 (1–2 marks)** Correct determination of empirical formula and/or molecular formula. **OR** Analyses some of the IR and NMR data. **OR** Analyses most of the NMR data.	**6**	**3.1× 4** **3.2× 2**	**Indicative scientific points:** **Empirical and Molecular Formulae** $= \frac{C}{56.69/12.0} : \frac{H}{7.09/1.0} : \frac{N}{11.02/14.0} : \frac{O}{25.20/16.0}$ **OR** 4.72 : 7.09 : 0.787 : 1.575 = 6 : 9 : 1 : 2 • Empirical formula = $C_6H_9NO_2$ • *m/z* = 127.0 and empirical formula mass (127) used to determine molecular formula as $C_6H_9NO_2$ **Structures of compound I**  **OR**  **OR**  **OR**  **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous

Mark Scheme

Question		Answer	Marks	AO element	Guidance
		There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant. **0 marks** No response or no response worthy of credit.			**Key features** • C ≡N • C=O in aldehyde, ketone, ester, amide, acid anhydride • CH_3 group that would give a doublet • CH_3 group that would give a triplet • CH_2 group that would give a quartet **^{1}H NMR and IR analysis** ^{1}H NMR spectrum • δ = 4.2 ppm, quartet, 2H CH_3–**CH_2**–O • δ = 2.9 ppm, quartet, 1H CO–**CH**–CH_3 • δ = 1.7 ppm, doublet, 3H CO–CH–**CH_3** • δ = 1.3 ppm, triplet, 3H **CH_3**–CH_2 IR spectrum • peak at 1750 (cm^{-1}) is C=O • peak at 2280 (cm^{-1}) is C ≡N **ALLOW** ranges from *Data Sheet* **IGNORE** references to C–O peaks