# GCE

## Chemistry A

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

Advanced GCE

# Mark Scheme for November 2020

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

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

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

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## 1. Annotations available in RM Assessor

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

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

| Annotation | Meaning |
|---|---|
| **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 |

1. **Subject-specific Marking Instructions**

**INTRODUCTION**

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

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

You should ensure that you have copies of these materials.

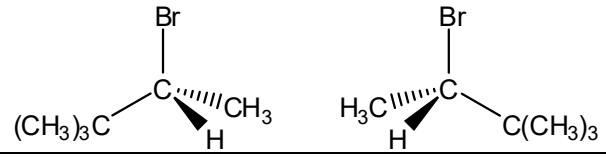
You should ensure also that you are familiar with the administrative procedures related to the marking process. These are set out in the OCR booklet **Instructions for Examiners**. If you are examining for the first time, please read carefully **Appendix 5 Introduction to Script Marking: Notes for New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

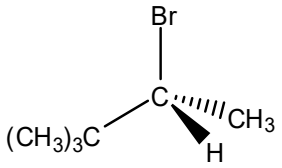
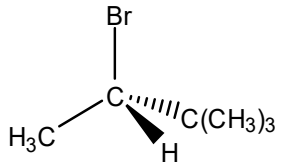
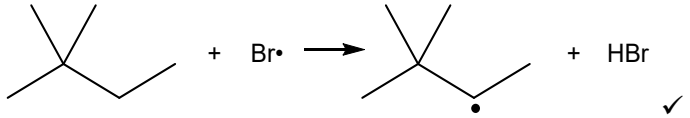
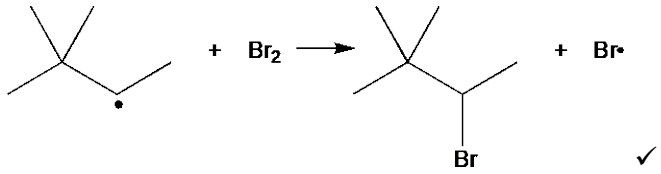
Please ask for help or guidance whenever you need it. Your first point of contact is your Team Leader.

**SECTION A**

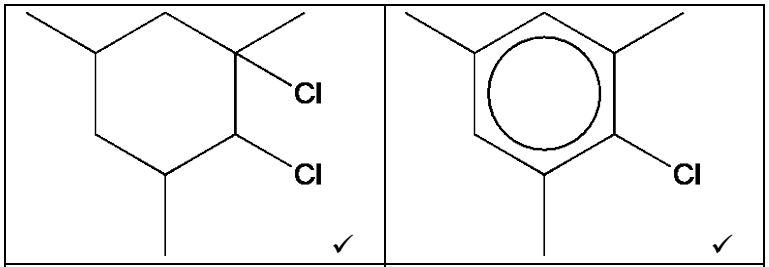
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|---|---|---|---|---|
| 1 | A | 1 | 1.2 | |
| 2 | B | 1 | 1.1 | |
| 3 | A | 1 | 1.1 | |
| 4 | C | 1 | 2.3 | |
| 5 | D | 1 | 1.2 | |
| 6 | D | 1 | 2.1 | |
| 7 | A | 1 | 1.1 | |
| 8 | C | 1 | 2.2 | |
| 9 | D | 1 | 1.2 | |
| 10 | C | 1 | 2.5 | ALLOW 5 |
| 11 | A | 1 | 2.6 | |
| 12 | A | 1 | 2.2 | |
| 13 | A | 1 | 1.1 | |
| 14 | B | 1 | 2.3 | |
| 15 | C | 1 | 1.2 | |

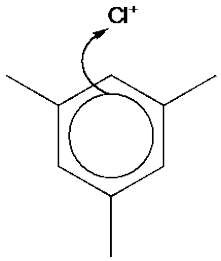
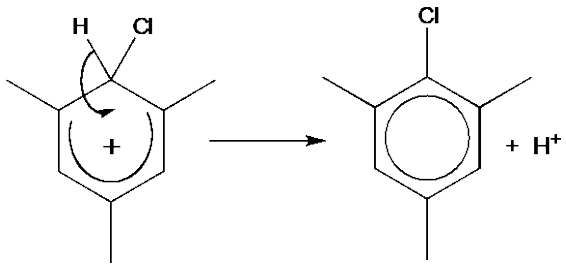
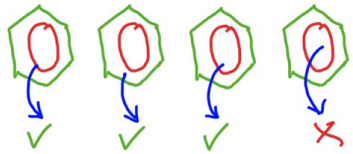
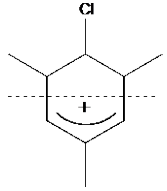
**SECTION B**

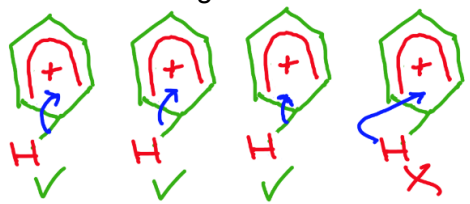
| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| 16 | (a) | (i) | 2-bromo-3,3-dimethylbutane ✓ | 1 | 1.2 | **IGNORE** lack of hyphens or addition of commas<br><br>**ALLOW** 3,3-dimethyl-2-bromobutane<br><br>**DO NOT ALLOW**<br>2-bromo-3-dimethylbutane<br>methy for methyl<br>methly for methyl<br>brom for bromo |
| | (b) | (i) | **Stereoisomers**<br>Same structural formula<br>**AND**<br>Different arrangement (of atoms) in space<br>**OR** different spatial arrangement (of atoms)<br>**AND**<br>**Type:** Optical ✓ | 1 | 1.2 | **ALLOW** structure/displayed/skeletal formula<br><br>**DO NOT ALLOW** same empirical formula<br>**OR** same general formula<br><br>**IGNORE** same molecular formula<br>**IGNORE** references to chiral molecules/compounds |
| | | (ii) | One 3D structure with correct groups attached to the chiral C ✓<br><br>Two 3D structures of $(CH_3)_3CCHBrCH_3$ that are mirror images **AND** correct connectivity in both ✓<br><br><br> | 2 | 2.5<br><br>1.2 | **ALLOW** small slip in one of the groups OR use of $C_4H_9$<br>3D structures must have four central bonds with **at least two wedges.**<br><br>For bond into paper accept:<br><br><br>**ALLOW** two 3D structures with 2 groups swapped e.g. |

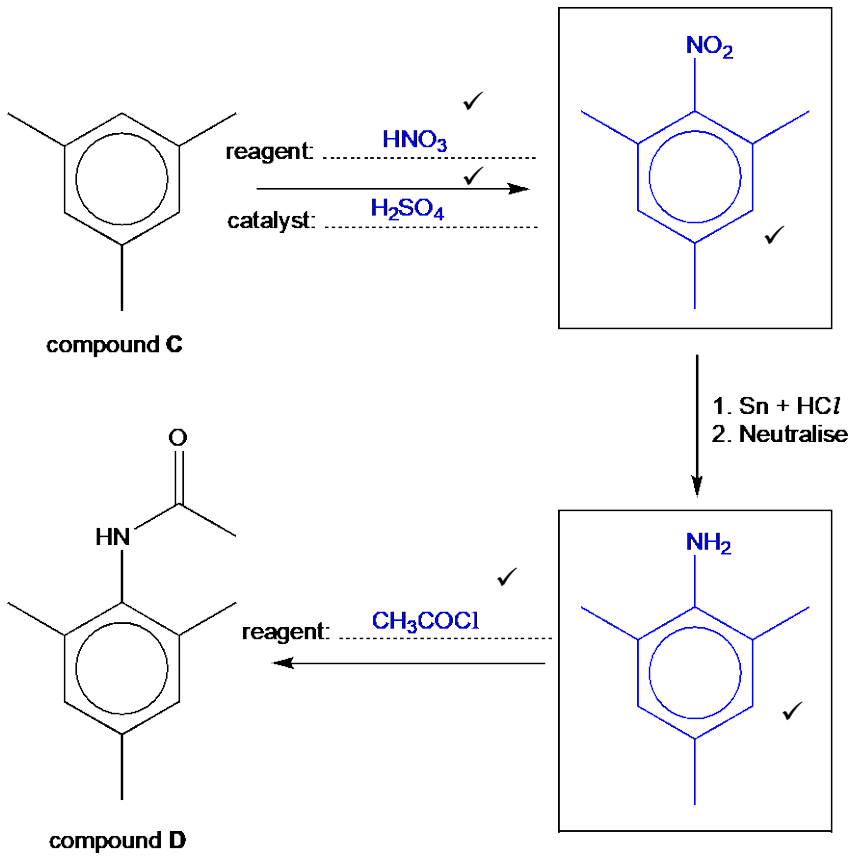
| Question | | | Answer | Marks | AO element | Guidance |
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| | | |     | | | |
| | (c) | | **Initiation**<br>$Br_2 \rightarrow 2Br\bullet$ ✓<br><br>**Propagation**<br>  ✓<br>  ✓ | 3 | 1.2<br><br>2.5×2 | **ALLOW** $Br_2 \rightarrow Br\bullet + Br\bullet$<br>**IGNORE** dots for initiation step,<br>i.e. **ALLOW** $Br_2 \rightarrow Br + Br$ **OR** $Br_2 \rightarrow 2Br$<br><br>**DOT REQUIRED** at correct position on chain.<br><br>**ALLOW 1 mark** if both propagation equations are correct by atom but dot(s) missing or on incorrect C in chain<br><br>**ALLOW 1 mark** if both propagation equations are correct including position of dot(s) but structures are not shown using skeletal formula<br><br>**ALLOW** ECF from incorrect intermediate |

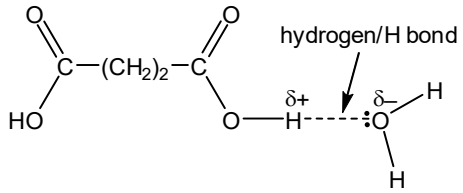
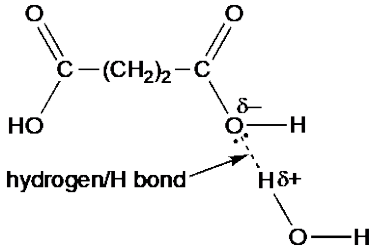
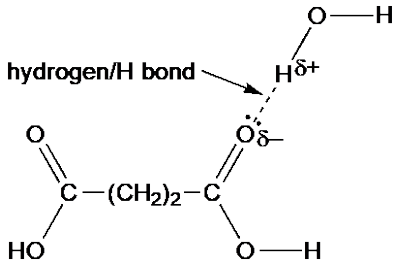
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| | (d) | | further substitution/s<br>**OR**<br>produces different termination products<br>**OR**<br>More than one termination step<br>**OR**<br>Mixture of products are formed ✓<br><br>substitution at different positions along chain ✓ | **2** | **1.1×2**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

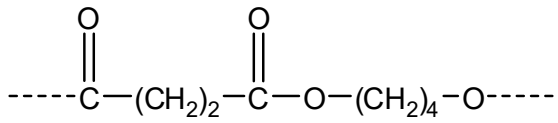
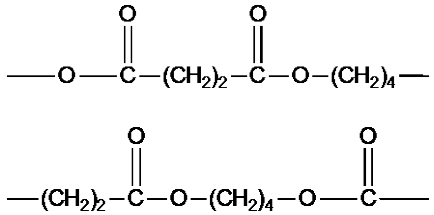
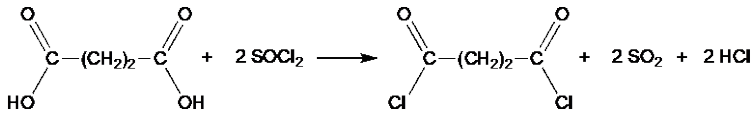
| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| 17 | (a) | (i) |  ✓ ✓<br>Organic product with **B** \| Organic product with **C** | **2** | **2.5×2** | |
| | | **(ii)** | **Reactivity of B**<br>in B electrons are localised<br>OR<br>in B π-bond is localised ✓<br><br>**Reactivity of C**<br>in C electrons are delocalised<br>OR<br>In C π-system / ring is delocalised<br><br>In **B**, electron density is higher<br>**AND**<br>B is more susceptible to electrophilic attack<br>**OR**<br>B attracts/accepts the electrophile/$Cl_2$ more<br>**OR**<br>B polarises the electrophile/$Cl_2$ more ✓<br>**ORA** | **3** | **1.1×3** | **ALLOW** labelled diagram to show delocalised system<br><br>**IGNORE** charge density<br>**IGNORE** electronegativity<br><br>**IGNORE** B is more reactive/reacts more readily (no reference to electrophile)<br><br>**IGNORE** references to electron density spread around the π–ring<br><br>**ALLOW** chlorine |

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

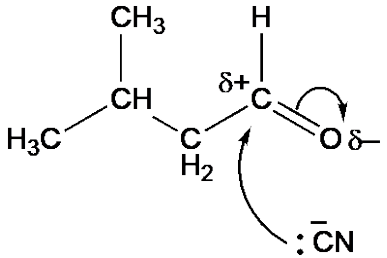
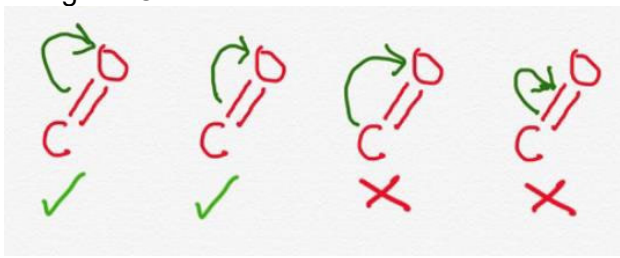
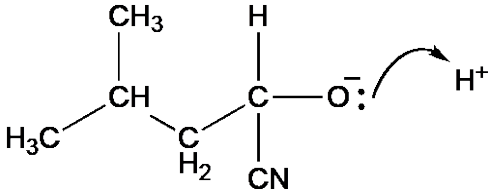
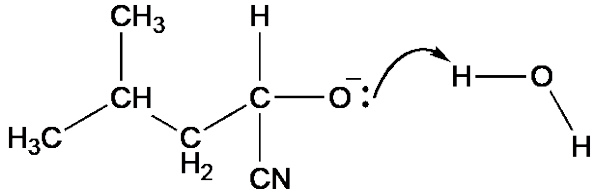
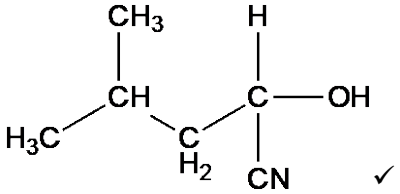
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<tr><th colspan="3">Question</th><th>Answer</th><th>Marks</th><th>AO element</th><th>Guidance</th></tr>
<tr><td></td><td></td><td></td><td></td><td></td><td></td><td>IGNORE partial charges on the chlorine in the intermediate<br><br>DO NOT ALLOW mark for intermediate if any $CH_3$ is missing<br><br>Curly arrow must start from, OR be traced back to, any part of C-H bond and go inside the ‘hexagon’<br><br><br>ALLOW use of $AlCl_4^-$ in the mechanism<br><br>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>$3C_3H_6O \rightarrow C_9H_{12} + 3H_2O$<br><br>molecular formulae of $C_3H_6O$ AND $C_9H_{12}$ ✓<br><br>$H_2O$ as by-product ✓<br><br>correct balanced equation ✓</td><td>3</td><td>2.6<br><br>2.5<br><br>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>
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| 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<br><br>**IGNORE** names for organic intermediates (question asks for structures<br><br>**ALLOW** names of reagents and catalyst<br><br>Around top arrow, **ALLOW** 1 of 2 marks if $HNO_3$ and $H_2SO_4$ swapped.<br>i.e.<br>reagent: $H_2SO_4$<br>catalyst: $HNO_3$<br><br>**IGNORE** references to concentration<br><br>**ALLOW** $(CH_3CO)_2O$ for left arrow<br><br>**IGNORE** $CH_3COOH$<br>**IGNORE** acyl chloride<br><br>**DO NOT ALLOW** $AlCl_3/FeCl_3$/Fe4 |

| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| 18 | (a) | (i) | **Reagents**<br>$K_2Cr_2O_7$ **AND** acid<br>**AND** reflux ✓<br><br>**Equation**<br>$HO(CH_2)_4OH + 4[O] \rightarrow HOOC(CH_2)_2COOH + 2H_2O$<br><br>[O] **AND** $H_2O$ ✓<br><br>Correctly balanced equation ✓ | **3** | <br><br>**1.1**<br><br><br><br>**2.5**<br><br>**2.6** | **ALLOW** $Na_2Cr_2O_7$ **OR** $Cr_2O_7^{2-}$<br>**ALLOW** $H_2SO_4$ **OR** HCl **OR** $H^+$<br>**ALLOW** words. e.g. 'acidified dichromate'<br>**ALLOW** a small slip in formula for dichromate e.g $KCr_2O_7$, |
| | | (ii) | <br><br>**OR**<br><br><br>Diagram showing correct dipole charges on each end of one hydrogen bond between a water molecule and a diacid ✓<br><br>Hydrogen bond between one lone pair on O atom in one of the molecules and the H atom of another<br>**AND**<br>Hydrogen bonding stated or labelled on diagram | **2** | **2.1×2** | **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous<br><br>**DO NOT ALLOW** δ+ on H atoms of $CH_2$ group<br><br>**ALLOW** H-bond for hydrogen bond<br><br>**ALLOW** H bond between C=O and $H_2O$, i.e.<br><br><br><br>**IF** diagram is not labelled, **ALLOW** hydrogen bond/H bond from text |

| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| | (b) | (i) | <br>Ester link (must be displayed) ✓<br>Rest of structure ✓ | 2 | 1.2<br>2.5 | **ALLOW** the 'O' or C=O at either end, e.g.<br><br>**IGNORE** brackets<br>**IGNORE** *n*<br>End bonds' **MUST** be shown (solid or dotted)<br>**DO NOT ALLOW** more than one repeat unit |
| | | (ii) | the ester/ ester bond/ ester group /polyester can be broken down ✓<br>**OR**<br>It can be hydrolysed ✓ | 1 | 3.2 | **IGNORE** references to photodegradable<br>'Bond breaks' is not sufficient – no reference to ester bond |
| | | (iii) | <br>$SOCl_2$ in equation ✓<br>Structure of diacyl dichloride ✓<br>Complete balanced equation ✓ | 3 | 1.1<br>1.2<br>2.6 | **ALLOW** alternative approach using $PCl_5$ or $PCl_3$ |

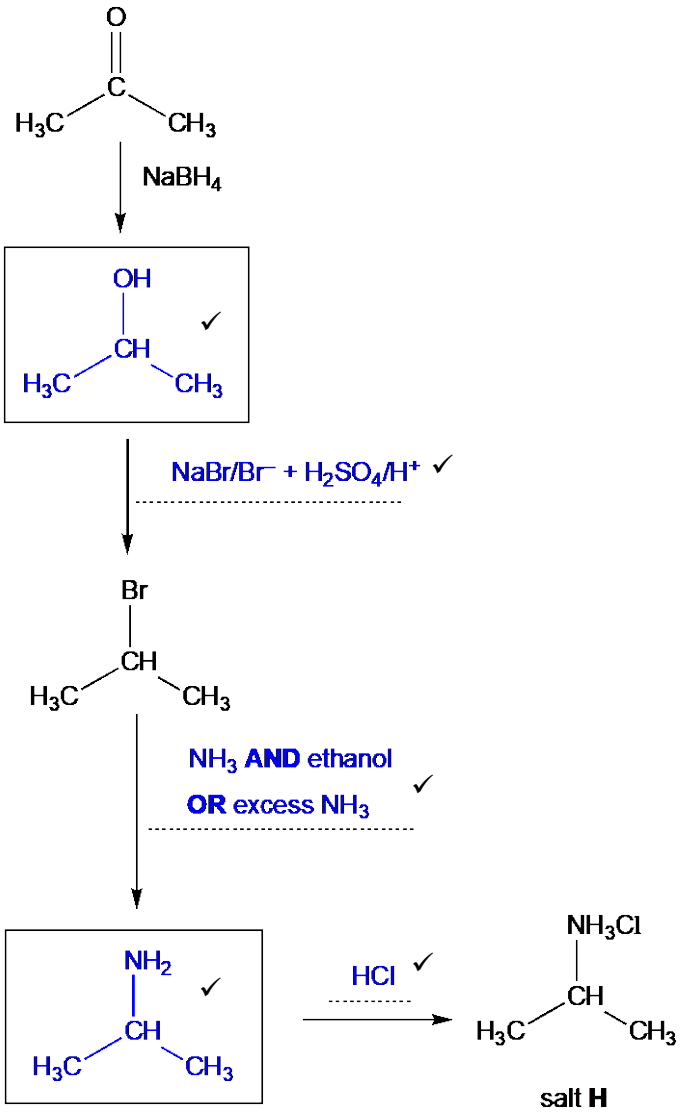
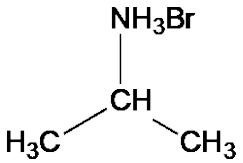
| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| 19 | (a) | (i) | (series of organic compounds with the) same functional group **OR** same/similar chemical properties/reactions ✓<br><br>each **successive/subsequent** member differs by $CH_2$ ✓ | 2 | 1.1 ×2 | **IGNORE** reference to physical properties<br>**IGNORE** same general formula<br>**DO NOT ALLOW** same empirical **OR** molecular formula<br>Differs by $CH_2$ is **not** sufficient (*no successive*) |
| | | (ii) | $C_{24}H_{48}O$ ✓ | 1 | 2.1 | |
| | (b) | | F/aldehyde<br>**AND**<br>Tollens' (reagent)<br>**AND**<br>Silver (mirror/precipitate/ppt/solid) ✓<br><br>G/alkene/C=C<br>**AND**<br>Bromine/$Br_2$<br>**AND**<br>goes colourless/decolourised ✓<br><br>G/ketone<br>**AND**<br>2,4-dinitrophenylhydrazine<br>**AND**<br>orange/yellow/red precipitate ✓<br><br>G/ketone<br>**AND**<br>Tollens' (reagent)<br>**AND**<br>no silver mirror/no change/no reaction ✓ | 4 | 2.3<br><br>3.3<br><br>3.3<br><br>3.3 | **IGNORE** use of 2,4-DNP with F<br><br>**ALLOW** ammoniacal silver nitrate **OR** $Ag^+/NH_3$<br>**ALLOW** black ppt **OR** grey ppt<br><br>**ALLOW** bromine water/ $Br_2(aq)$<br><br>**ALLOW** errors in spelling for 2,4-DNP<br>**ALLOW** 2,4(-)DNP **OR** 2,4(-)DNPH<br>**ALLOW** Brady's reagent or Brady's Test<br>**ALLOW** solid **OR** crystals **OR** ppt as alternatives for precipitate<br><br>**ALLOW** ammoniacal silver nitrate **OR** $Ag^+/NH_3$<br>**ALLOW** black ppt **OR** grey ppt<br><br>**ALLOW** alterative approach using acidified potassium dichromate for tests with F and/or G, with correct observations, alongside use of 2,4-DNP |

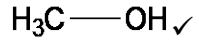
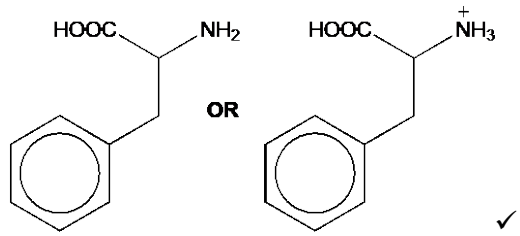
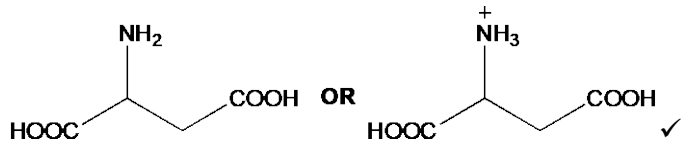
| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| | (c) | (i) | **Mechanism** ***3 marks*** | **5** | | **ANNOTATE ANSWER WITH TICKS AND CROSSES** |
| | | |  | | | Curly arrow must come from lone pair on C of $^{-}$CN **OR** $CN^{-}$ **OR** from minus sign on C of $^{-}$CN ion (then lone pair on $CN^{-}$ does not need to be shown) |
| | | | Curly arrow from $^{-}$CN to C atom of C=O ✓ | | **1.2** | Curly arrow from C=O bond must start from, OR be traced back to, any part of C=O bond and go to O |
| | | | Dipole shown on C=O bond, $C^{\delta+}$ and $O^{\delta-}$, **AND** curly arrow from C=O bond to O atom ✓ | | **1.2** |  |
| | | |  | | | ---------- |
| | | | Curly arrow from lone pair **OR** – charge on $O^{-}$ of **correct** intermediate to $H^{+}$ ✓ | | **2.5** | **ALLOW** curly arrow to H atom of $H_2O$, i.e. |
| | | | ---------- | | |  |
| | | | **Product** ***1 mark*** | | | **IGNORE** attempt to draw curly arrow showing breaking of H–O in $H_2O$ |
| | | |  ✓ | | **2.5** | |
| | | | ---------- | | | **IGNORE** lack of dipole on $H_2O$ |
| | | | **Name of mechanism** ***1 mark*** | | | |
| | | | Nucleophilic addition ✓ | | **1.1** | |

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

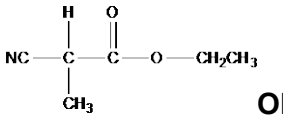
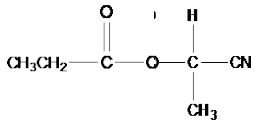
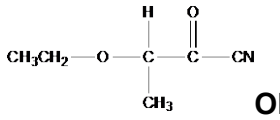
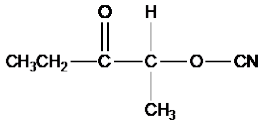
| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| 20 | (a)* | | *Refer to marking instructions on page 4 of mark scheme for guidance on marking this question.*<br><br>**Level 3 (5-6 marks**)<br>A correct calculation of the mass of cyclopentanol<br>**AND**<br>A **detailed** description of most purification steps<br><br>*There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.*<br><br>**Level 2 (3-4 marks)**<br>Calculates the mass of cyclopentanol with some errors<br>**AND**<br>A **detailed** description of some purification steps<br>**OR**<br>A correct calculation of the mass of cyclopentanol<br>**AND**<br>A **detailed** description of a few purification steps<br><br>*There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.*<br><br>**Level 1 (1-2 marks)**<br>Calculates the mass of cyclopentanol with some errors<br>**OR**<br>A **detailed** description of some purification steps<br><br>*There is an attempt at a logical structure with a line of reasoning. The information is in the most part relevant.*<br><br>**0 marks** No response or no response worthy of credit. | **6** | **2.8×2**<br>**3.3×4** | **Indicative scientific points may include:**<br>**<u>Calculation of mass of cyclopentanol</u>**<br>**Using moles**<br>• $n$(cyclopentene) = $\frac{4.00}{68}$ = 0.0588…. (mol)<br>• $n$(cyclopentanol) = 0.0588 × $\frac{100}{64}$ = 0.0919…(mol)<br>• Mass of cyclopentanol = 86 × 0.0919 = **7.90** g<br><br>**Using mass**<br>• Theoretical mass cyclopentene= 4.00 × $\frac{100}{64}$ = 6.25 g<br>• Theoretical $n$(cyclopentanol) = $\frac{6.25}{68}$ = 0.0919 (mol)<br>• Mass of cyclopentanol = 86 × 0.0919 = **7.90** g<br><br>**ALLOW** for small slip in Mr / rounding errors<br><br>**<u>Examples of some calculation errors</u>**<br>**Incorrect inverse ratio**:<br>• 0.0588 × $\frac{64}{100}$ = 0.0376…. (mol)<br>• Mass = 86 × 0.0376 = 3.24 g<br><br>**Ignoring % yield gives**:<br>• $\frac{4.00}{68}$ = 0.0588…. (mol)<br>• Mass = 86 × 0.0588 = 5.06 g<br><br>**<u>Purification</u>**<br>• Add a neutralising agent **by formula or name** e.g. $Na_2CO_3$<br>• In separating funnel, **organic layer is on top**<br>• Drying with an **anhydrous salt by formula or name**, e.g. $MgSO_4$, $Na_2SO_4$, $CaCl_2$<br>• Redistil **at approx. 44ºC**<br>**Examples** of detail in **bold** (**NOT INCLUSIVE**) |

| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| | (b) | | C=C/alkene peak in region 1620-1680 $cm^{-1}$ ✓<br><br>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<br><br>**IGNORE** references to C-O at 1000$cm^{-1}$ |

| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| 21 | (a) | |  | **5** | **2.5×5** | **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous<br><br>**ALLOW** HBr<br><br>**ALLOW** for the bottom left structure<br> |

| Question | | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|---|
| | (b) | (i) | Ester<br>Amide<br>Amine<br>Carboxylic acid<br>4 groups correct ✓✓✓<br>3 groups correct ✓✓<br>2 groups correct ✓ | 3 | 1.2×3 | **IGNORE** amino acid<br><br>**ALLOW** carboxyl<br><br>**IGNORE** attempt to classify amide, e.g. secondary<br>**IGNORE** formulae (question asks for names)<br><br>**IF > 4** functional groups are shown,<br>• Count 4 groups max but incorrect groups **first**<br><br>**IGNORE** aryl **OR** alkyl group<br>e.g. benzene, phenyl, aryl, arene, methyl |
| | | (ii) | **Methanol 1 mark**<br><br><br>**Amino Acids 3 marks**<br><br><br><br>Both amino acids shown with $NH_3^+$ ✓ | 4 | 2.5×4 | **ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous<br><br>**ALLOW** + charge on H of $NH_3$ group, i.e.$NH_3^+$<br><br>If **BOTH** amino acids are shown with $NH_3$ groups (without the + charge) **OR** as $NH_2^+$ groups, award 2 of the 3 marks for the amino acids<br><br>If **BOTH** amino acids are shown as correctly balanced salts, e.g $NH_3Cl$, all marks can be awarded. |

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

| Question | | Answer | Marks | AO element | Guidance |
|---|---|---|---|---|---|
| 22 | (a) | $CDCl_3$ used as a solvent ✓<br><br>$D_2O$ used to identify OH **OR** NH protons ✓ | 2 | 1.1×2 | Example and use required for each mark<br><br>**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.*<br><br>**Level 3 (5–6 marks)**<br>Structure **I** has a viable chemical structure of $C_6H_9NO_2$ which has the key features consistent with spectral data<br>**AND**<br>Most of the data analysed<br><br>*There is a well-developed line of reasoning which is clear and logically structured. The information presented is relevant and substantiated.*<br><br>**Level 2 (3–4 marks)**<br>Compound **I** has a viable chemical structure of $C_6H_9NO_2$ with most of the key features consistent with spectral data<br>**AND**<br>Some of the spectral data analysed.<br><br>*There is a line of reasoning presented with some structure. The information presented is relevant and supported by some evidence.*<br><br>**Level 1 (1–2 marks)**<br>Correct determination of empirical formula and/or molecular formula.<br>**OR**<br>Analyses some of the IR and NMR data.<br>**OR**<br>Analyses most of the NMR data. | 6 | 3.1× 4<br>3.2× 2 | **Indicative scientific points:**<br>**Empirical and Molecular Formulae**<br>$= \frac{C}{56.69/12.0} : \frac{H}{7.09/1.0} : \frac{N}{11.02/14.0} : \frac{O}{25.20/16.0}$<br>**OR** 4.72 : 7.09 : 0.787 : 1.575<br>= 6 : 9 : 1 : 2<br><br>• Empirical formula = $C_6H_9NO_2$<br>• *m/z* = 127.0 and empirical formula mass (127) used to determine molecular formula as $C_6H_9NO_2$<br><br>**Structures of compound I**<br><br> **OR** <br><br>**OR**<br><br> **OR** <br><br>**ALLOW** any combination of skeletal **OR** structural **OR** displayed formula as long as unambiguous |

| 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.*<br><br>**0 marks** No response or no response worthy of credit. | | | **Key features**<br>• C ≡N<br>• C=O in aldehyde, ketone, ester, amide, acid anhydride<br>• $CH_3$ group that would give a doublet<br>• $CH_3$ group that would give a triplet<br>• $CH_2$ group that would give a quartet<br><br>**$^1$H NMR and IR analysis**<br>$^1$H NMR spectrum<br>• δ = 4.2 ppm, quartet, 2H $CH_3$–**$CH_2$**–O<br>• δ = 2.9 ppm, quartet, 1H CO–**CH**–$CH_3$<br>• δ = 1.7 ppm, doublet, 3H CO–CH–**$CH_3$**<br>• δ = 1.3 ppm, triplet, 3H **$CH_3$**–$CH_2$<br><br>IR spectrum<br>• peak at 1750 ($cm^{-1}$) is C=O<br>• peak at 2280 ($cm^{-1}$) is C ≡N<br>**ALLOW** ranges from *Data Sheet*<br>**IGNORE** references to C–O peaks |

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