

Mark Scheme (Results)

Summer 2015

IAL Chemistry (WCH04)

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General Marking Guidance

- All candidates must receive the same treatment. Examiners must mark the first candidate in exactly the same way as they mark the last.
- Mark schemes should be applied positively. Candidates must be rewarded for what they have shown they can do rather than penalised for omissions.
- Examiners should mark according to the mark scheme not according to their perception of where the grade boundaries may lie.
- There is no ceiling on achievement. All marks on the mark scheme should be used appropriately.
- All the marks on the mark scheme are designed to be awarded. Examiners should always award full marks if deserved, i.e. if the answer matches the mark scheme. Examiners should also be prepared to award zero marks if the candidate's response is not worthy of credit according to the mark scheme.
- Where some judgement is required, mark schemes will provide the principles by which marks will be awarded and exemplification may be limited.
- When examiners are in doubt regarding the application of the mark scheme to a candidate's response, the team leader must be consulted.
- Crossed out work should be marked UNLESS the candidate has replaced it with an alternative response.
- Mark schemes will indicate within the table where, and which strands of QWC, are being assessed. The strands are as follows:
 - i) ensure that text is legible and that spelling, punctuation and grammar are accurate so that meaning is clear
 - ii) select and use a form and style of writing appropriate to purpose and to complex subject matter
 - iii) organise information clearly and coherently, using specialist vocabulary when appropriate

Section A (multiple choice)

Question Number	Correct Answer	Mark
1	A	1

Question Number	Correct Answer	Mark
2	C	1

Question Number	Correct Answer	Mark
3	A	1

Question Number	Correct Answer	Mark
4	C	1

Question Number	Correct Answer	Mark
5	C	1

Question Number	Correct Answer	Mark
6(a)	D	1

Question Number	Correct Answer	Mark
6(b)	B	1

Question Number	Correct Answer	Mark
7	B	1

Question Number	Correct Answer	Mark
8(a)	D	1

Question Number	Correct Answer	Mark
8(b)	C	1

Question Number	Correct Answer	Mark
9	B	1

Question Number	Correct Answer	Mark
10(a)	C	1

Question Number	Correct Answer	Mark
10(b)	A	1

Question Number	Correct Answer	Mark
10(c)	D	1

Question Number	Correct Answer	Mark
11(a)	D	1

Question Number	Correct Answer	Mark
11(b)	C	1

Question Number	Correct Answer	Mark
11(c)	A	1

Question Number	Correct Answer	Mark
12(a)	B	1

Question Number	Correct Answer	Mark
12(b)	A	1

Question Number	Correct Answer	Mark
12(c)	B	1

Total for Section A = 20 marks

Section B

Question Number	Acceptable Answers	Reject	Mark
13(a) (i)	<p>1st mark: Identification of buffer</p> <p>Any mention of buffer solution / buffering (region) (1)</p> <p>2nd mark: Identification of species responsible for buffering action</p> <p>ammonia/NH₃ and ammonium ions /NH₄⁺ present (in significant concentrations) OR ammonia/NH₃ and ammonium chloride /NH₄Cl present (in significant concentrations) OR weak base and salt/conjugate acid present (in significant concentrations) OR B and BH⁺ present (in significant concentrations) Can be awarded from a correct equation (1)</p> <p>3rd mark: For mention of how this buffer works on addition of small amounts of H⁺ ions</p> <p>(relatively large concentration/reservoir of) ammonia molecules react with added hydrogen ions/ H⁺ /(hydrochloric) acid OR (relatively large concentration /reservoir of weak) base reacts with added hydrogen ions / H⁺ /(hydrochloric) acid OR H⁺ + NH₃ → NH₄⁺ Allow reversible arrow OR Adding (hydrochloric) acid/H⁺ /hydrogen ions has negligible effect on ratio [NH₃]:[NH₄⁺] (1)</p> <p>Ignore references to buffering action on addition of OH⁻ (not relevant here)</p> <p>Ignore general descriptions of buffer solution eg resists change in pH when small amounts of acid or alkali added</p>	<p>Acidic buffer</p> <p>Weak acid and its conjugate base HA and A⁻</p>	3

Question Number	Acceptable Answers	Mark
13(a) (ii)	<p>Note – the equations $\text{NH}_4^+ + \text{H}_2\text{O} \rightarrow \text{NH}_3 + \text{H}_3\text{O}^+$ $\text{NH}_4^+ + \text{H}_2\text{O} \rightarrow \text{NH}_4\text{OH} + \text{H}^+$ score all three marks</p> <p>Note –the equation $\text{NH}_4^+ \rightarrow \text{NH}_3 + \text{H}^+$ scores 2 marks, but if (aq) state symbols are given, scores 3 marks</p> <p>1st mark: Ammonium ions /NH_4^+ present (at equivalence point) OR ammonium chloride/ammonium salt (1)</p> <p>2nd mark Ammonium (ions) / NH_4^+ react with water /hydrolysed by water /dissociate in water Ignore ammonium chloride reacts with water (1)</p> <p>3rd mark $\text{NH}_4^+ \rightarrow \text{NH}_3 + \text{H}^+$ OR $\text{NH}_4^+ + \text{H}_2\text{O} \rightarrow \text{NH}_3 + \text{H}_3\text{O}^+$ Allow $\text{NH}_4^+ + \text{H}_2\text{O} \rightarrow \text{NH}_4\text{OH} + \text{H}^+$ (1)</p> <p>Note if no other mark awarded Just 'strong acid – weak base (titration)' / ammonium chloride is the salt of a strong acid and a weak base scores (1) only</p>	3

Question Number	Acceptable Answers	Mark
13(a)(iii)	<p>If final answer is 1.6(2), with correct working or without working, award 4 marks</p> <p>Mol of ammonia used = $(25/1000 \times 0.024)$ $= 6 \times 10^{-4}$ mol</p> <p>and</p> <p>Mol of acid added = $(40/1000 \times 0.054)$ $= 2.16 \times 10^{-3}$ (1)</p> <p>Mol of excess acid = $2.16 \times 10^{-3} - 6 \times 10^{-4}$ $= 1.56 \times 10^{-3}$ mol (1)</p> <p>$[H^+] = 1.56 \times 10^{-3} / (65/1000) = 0.024$ mol dm⁻³ (1)</p> <p>pH = $-\log [H^+] = 1.6(2)$ (1)</p> <p>Ignore SF except 1 SF Allow TE for 2nd, 3rd marks Allow TE for 4th mark provided pH is less than 7 and it is based on some use of data in question</p> <p>Alternative method for 1st and 2nd marks</p> <p>Mol of ammonia used = $(25/1000 \times 0.024)$ $= 6 \times 10^{-4}$ mol</p> <p>and</p> <p>Volume of acid used = $\frac{6 \times 10^{-4} \times 1000}{0.054}$ $= 11.111$ cm³ (1)</p> <p>Volume of acid left = $40 - 11.111$ $= 28.889$ cm³</p> <p>Mol of excess acid = $\frac{28.889 \times 0.054}{1000}$ $= 1.56 \times 10^{-3}$ mol (1)</p>	4

Question Number	Acceptable Answers	Reject	Mark
13(b)(i)	<p>EITHER</p> <p>$[H^+]^2 = 5.5 \times 10^{-13}$ or $[H^+] = \sqrt{5.5 \times 10^{-13}}$ / 7.416×10^{-7} (mol dm⁻³) (1)</p> <p>pH = $-\log \sqrt{5.5 \times 10^{-13}}$ (= 6.12982 / 6.13) (1)</p> <p>OR</p> <p>pK_w = 12.26 (1)</p> <p>pH = $\frac{1}{2}$ pK_w (= 6.130) (1)</p>	6.13 with no working	2

Question Number	Acceptable Answers	Reject	Mark
13(b) (ii)	Neutral (1) $[H^+] = [OH^-]$ /equal amounts of H^+ and OH^- ions OR Both $[H^+]$ and $[OH^-]$ have increased by the same amount (1)	Acidic or alkaline for both marks	2

Total for Question 13 = 14 marks

Question Number	Acceptable Answers	Reject	Mark
14(a)	<p>The first two marks can be scored from a diagram or a written account</p> <p>Suitable reaction vessel e.g. side arm conical flask / flask with delivery tubing attached via bung / side arm boiling/test tube / boiling/test tube with delivery tubing attached via bung (1)</p> <p>Method of gas collection e.g. gas syringe / upturned measuring cylinder/burette over water Allow this as a label on a poorly drawn diagram (1)</p> <p>Measure volume collected at time intervals / time taken to collect fixed volume Allow mention of volume and time Allow amount of gas and time Ignore measure time taken for reaction to go to completion (1)</p> <p>OR A suitable open reaction vessel (but plugged with cotton wool) (1)</p> <p>Use of balance (1)</p> <p>Measure the mass at various time intervals / at a fixed time on a balance Allow mention of mass (loss) and time (1)</p> <p>Ignore heating</p>	<p>Diagram of apparatus that will not work eg delivery tube starting in solution or apparatus not sealed for first mark only</p> <p>Measure rate at which gas is produced</p>	3

Question Number	Acceptable Answers	Mark
14(b)(i)	<p>Any linked pair of responses. In each pair, the 2nd mark is dependent on the 1st mark being awarded.</p> <p>EITHER Reaction is endothermic /energy taken in / temperature falls Allow just "lower temperature" Ignore room temperature falls (1)</p> <p>Decreases rate of reaction (1)</p> <p>OR There is loss of product/gas before the apparatus is sealed (1)</p> <p>This is greater because the reaction is at a higher concentration (of A) (1)</p> <p>OR Active sites/surface (area) on catalyst full/blocked/saturated (1)</p> <p>Because the reaction is at a higher concentration (of A)/ decreases rate of reaction (1)</p> <p>Ignore references to experimental error</p> <p>Ignore comparisons of concentrations of A and B</p> <p>Ignore any reference to side-reactions</p>	2

Question Number	Acceptable Answers	Mark
14(b)(ii)	<p>0 order (1)</p> <p>As increase/change in concentration does not affect the rate /rate is independent of [A] Allow graph is a horizontal line / has zero gradient (1)</p> <p>Ignore graph is a straight line Ignore just 'there is no change in the rate' / 'rate is constant' / gradient remains constant</p>	2

Question Number	Acceptable Answers	Mark
14(c)(i)	<p>EITHER increases reliability improves validity (of the data obtained) / confirms the initial result / to check for anomalous results Ignore References to average/precision/accuracy</p> <p>OR to determine order w.r.t B and/or X / to determine order w.r.t reactants / substances / to find overall order / to see the effect of B and/or X on the rate/ to see the effect of reactants/ substances on the rate/ to determine rate equation / to calculate k</p> <p>Allow to find out which species are in the rate determining step</p>	1

Question Number	Acceptable Answers	Mark
14(c)(ii)	<p>2nd order w.r.t B (1)</p> <p>(Compare expt 1 & 2 when [X] is constant), as [B] triples so rate increases by a factor of 9 (1)</p> <p>First order w.r.t X (1)</p> <p>EITHER (using experiments 1 and 3 or 1 and 4) as [B] quadruples so rate should increase by a factor of 16 but increases by a factor of 32 / additional increase of x 2 due to doubling of [X] (hence first order w.r.t X)</p> <p>OR (using experiments 2 and 3 or 2 and 4) as [B] x4/3 (1.333) so rate should increase by a factor of 16/9 (1.778) but increases by 3.556 / additional increase of x2 due to doubling of [X] (hence first order w.r.t X)</p> <p>Allow these explanations shown as equations</p> <p>If C used instead of X, allow both marks for order and explanation (1)</p> <p>Allow TE on order w.r.t A and B</p>	4

Question Number	Acceptable Answers	Mark
14(c)(iii)	<p>Rate=$k[B]^2[X]$ / Rate=$k[A]^0[B]^2[X]$</p> <p>Allow r/R for rate and K for k</p> <p>Allow TE from b(ii) and c(ii)</p>	1

Question Number	Acceptable Answers	Mark
14(c)(iv)	<p>$k = \text{rate}/[B]^2[X] = 0.08/(0.1 \times 0.1 \times 0.2)$ $= 40$ (1)</p> <p>$\text{dm}^6\text{mol}^{-2}\text{s}^{-1}$ Allow units in any order (1)</p> <p>Allow use of data from experiments 1, 2 & 4</p> <p>Allow TE from c(iii)</p>	2

Question Number	Acceptable Answers	Mark
14(d)	<p>Correct feature – two from</p> <p>Mechanism does involve (formation of) a transition state Allow mechanism does involve the (formation of) an intermediate Allow transition/intermediate step (1)</p> <p>Second order overall / S_N2 /both halogenoalkane and hydroxide ions involves in slow step/rds/1st Step (1)</p> <p>Correct curly arrow from C-Br bond to Br (1)</p> <p>Transition state has a negative charge / correct charge Or Charges on all species are correct (1)</p> <p>Ignore references to stereochemistry Ignore references to final product correct/ lone pairs correct</p> <p>Incorrect features – two from</p> <p>Curly arrow should go from OH⁻ to carbon (attached to Br as it represents movement of a lone pair of electrons) / OH⁻ should give electrons rather than accept them Allow the arrow between C and O should be in the opposite direction (1)</p> <p>Bonds to OH and Br should be partial bonds /dotted lines (in transition state as insufficient electrons for (five) complete bonds) / carbon can only form four full bonds (1)</p> <p>Allow Dipole/partial charges on C-Br not shown (1)</p> <p>Ignore Mechanism should be 1 step not 2 steps for S_N2 Ignore there should be a curly arrow from C-Br bond to Br in the transition state</p>	4

Total for Question 14 = 19 marks

Question Number	Acceptable Answers	Reject	Mark
15(a)	ethyl dodecanoate Allow ethyldodecanoate ethyl dodecan-1-oate	ethyl decanoate / ethyl dodecanal/ ethyl dodecate / ethanoyl dodecanoate	1

Question Number	Acceptable Answers	Mark
15(b)	Reducing (agent) Allow (source of) nucleophile Ignore source of hydride ions	1

Question Number	Acceptable Answers	Mark
15(c)	Prevent further reduction / reduction of the aldehyde (to an alcohol) Allow to prevent further reaction of dodecanal /aldehyde Ignore reference to rates Ignore higher yield/ prevent side reactions Ignore exothermic / optimum temperature Ignore volatility	1

Question Number	Acceptable Answers	Mark
15(d)	<p>If final answer is 3.74 (g), with or without working, award 3 marks</p> <p>Moles ester = $5.26 / 228 = 0.02307$ mol NOTE: Do not allow this rounded to 0.02 (1)</p> <p>EITHER So mass of aldehyde at 100% = 0.02307×184 = 4.2449 (g) (1)</p> <p>But yield is 88%, so actual mass = 4.245×0.88 = 3.7355 / 3.74 (g) Allow 3.73 g if 4.24 g of aldehyde used (1)</p> <p>OR But yield is 88%, so actual moles = 0.02307×0.88 = 0.02(03) (1)</p> <p>So mass of aldehyde formed = 0.0203×184 = 3.7355 / 3.74 /3.7 (g) (1)</p> <p>Allow TE for 2nd and 3rd marks</p> <p>Ignore SF in final answer except 1SF</p>	3

Total for Question 15 = 6 marks

Question Number	Acceptable Answers	Reject	Mark
16(a)(i)	(fractional) distillation / steam distillation / solvent extraction Ignore filtration / use of separating funnel	recrystallisation	1

Question Number	Acceptable Answers	Mark
16(a)(ii)	$3\text{C}_{15}\text{H}_{31}\text{COOCH}_3 + \begin{array}{c} \text{CH}_2\text{OH} \\ \\ \text{CHOH} \\ \\ \text{CH}_2\text{OH} \end{array}$ 3 C ₁₅ H ₃₁ COOCH ₃ Allow 3 CH ₃ OOCC ₁₅ H ₃₁ Allow the correct formulae written three times (1) Correct formula for propane-1,2,3-triol (1) Mark independently	2

Question Number	Acceptable Answers	Mark
16(a)(iii)	Sodium hydroxide / potassium hydroxide / NaOH / KOH / OH ⁻ Allow sulfuric acid / H ₂ SO ₄ or other named strong acids or strong alkalis / HCl / just 'acid' / just 'base' / just 'alkali' / just H ⁺ Ignore concentrations of reagents, incorrect or missing state symbols	1

Question Number	Acceptable Answers	Mark
16(b)	<p>Do not award any marks for processing the plants or seeds into bio-diesel as the question is about growing</p> <p>Award (1) mark for any statement in the following headings:</p> <p>GREEN e.g. samphire / non-edible seeds / both are renewable / (produce bio-diesel that is) carbon neutral Ignore just "green / sustainable"</p> <p>LAND e.g. samphire uses land unlikely to be used for growing other food crops / no need to cut down trees to provide land / non-edible seed take up land otherwise used to grow crops</p> <p>WASTE e.g. non-edible seeds have no other use / would be thrown away / can only be used for oil production</p> <p>FOOD e.g. using samphire for bio-diesel reduces availability as a food source</p> <p>FOOD CHAIN e.g. using samphire disrupts the food chain for (marine) organisms</p> <p>GROWING e.g. samphire doesn't need to be irrigated / can take water or nutrients from the marshland Ignore just 'easier to grow' Ignore does not need specific conditions</p> <p>WEATHER e.g. samphire growing is subject to coastal weather</p> <p>TECHNOLOGY e.g. using samphire needs new / improved technology OR machines to farm coastal areas OR higher transport costs (from marshland to production plant) Ignore technology for processing plants or seeds</p> <p>WILL IT WORK? e.g. samphire gives unknown yield / use may need more research</p> <p>To score the maximum of 4 marks, the response must include a decision about which is greener but there is no separate mark for this.</p>	4

Total for Question 16 = 8 marks

Section C

Question Number	Acceptable Answers	Mark															
17(a)(i)	<table border="1"> <thead> <tr> <th></th> <th>CH₃CH₂CH₂CH₃</th> <th>O₂</th> <th>CH₃CO₂H</th> <th>H₂O</th> </tr> </thead> <tbody> <tr> <td>ΔH_f^\ominus / kJ mol⁻¹</td> <td>-126.5</td> <td>0</td> <td>-484.5</td> <td>-285.8</td> </tr> <tr> <td>S^\ominus / J mol⁻¹ K⁻¹</td> <td>310.1</td> <td>205</td> <td>159.8</td> <td>69.9</td> </tr> </tbody> </table> <p>6 values correct 3 marks</p> <p>4 / 5 values correct 2 marks</p> <p>2/3 values correct 1 mark</p> <p>0/1 values correct 0 marks</p> <p>Ignore values multiplied by balancing numbers in addition to correct values eg for water 2 x -285.8 (=571.6)</p>		CH ₃ CH ₂ CH ₂ CH ₃	O ₂	CH ₃ CO ₂ H	H ₂ O	ΔH_f^\ominus / kJ mol ⁻¹	-126.5	0	-484.5	-285.8	S^\ominus / J mol ⁻¹ K ⁻¹	310.1	205	159.8	69.9	3
	CH ₃ CH ₂ CH ₂ CH ₃	O ₂	CH ₃ CO ₂ H	H ₂ O													
ΔH_f^\ominus / kJ mol ⁻¹	-126.5	0	-484.5	-285.8													
S^\ominus / J mol ⁻¹ K ⁻¹	310.1	205	159.8	69.9													

Question Number	Acceptable Answers	Mark
17(a)(ii)	<p>If answer is - 2256.6 / - 2257 (kJ mol⁻¹), award 2 marks</p> <p>[(2 x -285.8) + (4 x -484.5)] - (2 x -126.5) (1)</p> <p>= - 2256.6 / - 2257 (kJ mol⁻¹) (1)</p> <p>Allow answer converted to J mol⁻¹</p> <p>Allow TE from incorrect data in table in (a)(i)</p> <p>Allow (1) for cycle wrong way round eg (+) 2256.6 / (+)2257 (kJ mol⁻¹)</p> <p>Allow (1) for using correct values but not multiplied by balancing numbers eg -643.8 (kJ mol⁻¹)</p> <p>Ignore SF except 1SF</p>	2

Question Number	Acceptable Answers	Mark
17(a) (iii)	<p>If answer is $-866.2 \text{ (J mol}^{-1}\text{K}^{-1}\text{)}$, award 2 marks</p> $\frac{[(2 \times 69.9) + (4 \times 159.8)] - [(2 \times 310.1) + (5 \times 205)]}{-866.2 \text{ (J mol}^{-1}\text{K}^{-1})}$ <p>(1)</p> <p>(1)</p> <p>Allow answer converted to $\text{kJ mol}^{-1}\text{K}^{-1}$</p> <p>Allow TE from incorrect data in table in (a)(i)</p> <p>Allow (1) for cycle wrong way round eg (+) $866.2 \text{ (J mol}^{-1}\text{K}^{-1}\text{)}$</p> <p>Allow (1) for using correct values but error(s) in balancing numbers eg $-285.4 \text{ (J mol}^{-1}\text{K}^{-1}\text{)}$</p> <p>Ignore SF except 1SF</p>	2

Question Number	Acceptable Answers	Mark
17(a) (iv)	<p>If answer is (+) $6706.3 \text{ J mol}^{-1} \text{ K}^{-1}$ or (+) $6.7063 \text{ kJ mol}^{-1} \text{ K}^{-1}$, award 3 marks</p> $\Delta S_{\text{surr}} \text{ at } 298 \text{ K} = -\Delta H/T$ $= -(-2256.6 \times 1000) / 298$ <p>(1)</p> $= 7572.483... \text{ (J mol}^{-1}\text{K}^{-1}\text{)}$ <p>Allow rounding to 3SF or more (1)</p> <p>Allow correct answers given in $\text{kJ mol}^{-1} \text{ K}^{-1}$ eg $7.5725 \text{ kJ mol}^{-1} \text{ K}^{-1}$</p> $\Delta S_{\text{tot}} = \Delta S_{\text{surr}} + \Delta S_{\text{sys}} / \Delta S_{\text{tot}} = -866.2 + 7572.5 / \Delta S_{\text{tot}} = (+)6706.3 \text{ J mol}^{-1} \text{ K}^{-1}$ <p>OR</p> $-0.8662 + 7.5725 / \Delta S_{\text{tot}} = (+)6.7063 \text{ kJ mol}^{-1} \text{ K}^{-1}$ <p>(1)</p> <p>Allow TE from (a)(ii) and (a)(iii)</p> <p>Ignore SF except 1SF in final answer</p>	3

Question Number	Acceptable Answers	Mark
17(a)(v)	<p>1st mark: consideration of ΔS_{system} ΔS_{sys} is not (significantly) changed /is unchanged /remains (approximately) constant (1)</p> <p>2nd mark: consideration of ΔS_{surr} (Higher temperature makes) $\Delta S_{\text{surr}} / -\Delta H/T$ is smaller / decreases / less positive Comment Allow more negative (1) No TE if ΔS_{surr} is -ve in (a)(iv)</p> <p>3rd mark: consideration of ΔS_{total} EITHER reduces ΔS_{tot} / makes ΔS_{tot} less positive / makes ΔS_{tot} closer to zero (so would not produce a greater yield)</p> <p>OR ΔS_{tot} is very large (so K is very large) so the effect of change in temperature is negligible (1)</p> <p>NOTE if ΔS_{surr} is -ve in (iv), then allow increases ΔS_{tot} / makes ΔS_{tot} more positive / makes ΔS_{tot} closer to zero (so would produce a greater yield).</p> <p>NOTE IF no reference / an incorrect reference made to ΔS_{system}, then only the 2nd and 3rd marks can be awarded</p>	3

Question Number	Acceptable Answers	Mark
17(b)	<p>Note: All we are looking for are the correct ranges, exactly as given below (i.e. the bonds do not have to be stated, as they follow from the correct ranges)</p> <p>Peak between 1725 – 1700 (cm^{-1}) (would appear due to C=O group (in alkyl carboxylic acid))</p> <p>Allow peak between 3300 – 2500 (cm^{-1}) (due to OH group (in carboxylic acid))</p>	1

Question Number	Acceptable Answers	Mark
17(c)	<p>increase sourness / sharpness of flavour</p> <p>OR preservative / prevents growth of microbes / prevents food decay / prevents food decomposition / kills microbes</p> <p>OR acidity regulator / buffer</p> <p>Allow improves flavouring</p> <p>Ignore reduce pH/ make (slightly) acidic/just 'flavouring'</p>	1

Question Number	Acceptable Answers	Mark
17(d)(i)	<p>Working must be shown</p> <p>EITHER % of oxygen = 40% (1)</p> <p>Amount of C = $52.5/12 = 4.375$ (mol) Amount of H = $7.5/1 = 7.5$ (mol) Amount of O = $40/16 = 2.5$ (mol) (1)</p> <p>Ratio 1.75 C : 3 H : 1 O $\equiv 7$ C : 12 H : 4 O Ignore SF in mol and ratios (1)</p> <p>OR % of C in $C_7H_{12}O_4 = \frac{84}{160} \times 100 = 52.5\%$ (1) % of H in $C_7H_{12}O_4 = \frac{12}{160} \times 100 = 7.5\%$ (1) % of O in $C_7H_{12}O_4 = \frac{64}{160} \times 100 = 40\%$ (1)</p> <p>OR No C atoms = $\frac{52.5 \times 160}{100 \times 12} = 7$ (1) No H atoms = $\frac{7.5 \times 160}{100 \times 1} = 12$ (1) No O atoms = $\frac{40 \times 160}{100 \times 16} = 4$ (1)</p>	3

Question Number	Acceptable Answers	Reject	Mark
17(d)(ii)	<p>Largest/highest m/e or m/z value (is 160) OR Mass (/charge ratio) or m/e or m/z of molecular/parent ion/ $C_7H_{12}O_4^+$ (=160(=M_r))</p> <p>Allow last peak / peak on rhs (is at 160)</p> <p>Allow peak before last (is at 160 due to M+1 peak at 161)</p>	<p>Highest peak</p> <p>Just 'there is a peak at 160'</p>	1

Question Number	Acceptable Answers	Mark																
17(d) (iii)	<p>For 'chemical shift' column, allow any range or any single value within range and allow range in the opposite order eg 3.0-1.8</p> <table border="1"> <thead> <tr> <th>Feature of compound X</th> <th>Chemical shift / ppm for TMS</th> <th>Splitting patterns</th> <th>Relative area below peak</th> </tr> </thead> <tbody> <tr> <td>CH₃</td> <td>0.1 – 1.9</td> <td>doublet</td> <td>3 (1)</td> </tr> <tr> <td>CH</td> <td>1.8 – 3.0 (1)</td> <td>septuplet / heptuplet / splits into 7 / 7 splits (1)</td> <td>1</td> </tr> <tr> <td>COOH</td> <td>10 – 12.0 (1)</td> <td>singlet</td> <td>1</td> </tr> </tbody> </table> <p>Allow heptet / septet / sevenlet and similar words that indicate 7</p>	Feature of compound X	Chemical shift / ppm for TMS	Splitting patterns	Relative area below peak	CH ₃	0.1 – 1.9	doublet	3 (1)	CH	1.8 – 3.0 (1)	septuplet / heptuplet / splits into 7 / 7 splits (1)	1	COOH	10 – 12.0 (1)	singlet	1	4
Feature of compound X	Chemical shift / ppm for TMS	Splitting patterns	Relative area below peak															
CH ₃	0.1 – 1.9	doublet	3 (1)															
CH	1.8 – 3.0 (1)	septuplet / heptuplet / splits into 7 / 7 splits (1)	1															
COOH	10 – 12.0 (1)	singlet	1															

Total for Question 17 = 23 marks

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