



## Mark Scheme

Q1.

| Question Number | Acceptable Answer  | Additional Guidance   | Mark |
|-----------------|--|---|------|
| (i)             | <ul style="list-style-type: none"> <li>relative abundance of missing isotope (<math>^{37}\text{Cl}</math>) (1)</li> <li>relative height of missing peak (1)</li> </ul>   | <p><u>Example of calculation</u></p> $(100 - 75.5) = 24.5$ $\frac{82.5 \times 24.5}{75.5} = 26.772$ <p>Ignore SF except 1 SF<br/>DNA incorrect rounding for M2<br/>Correct answer with no working scores (2)<br/>TE on M1</p>   | (2)  |
| Question Number | Acceptable Answer  | Additional Guidance   | Mark |
| (ii)            | <ul style="list-style-type: none"> <li>(there are) three (possible) combinations of the two isotopes in chlorine molecules/<math>\text{Cl}_2</math></li> </ul>   | <p>Allow a specific illustration using these 3 combinations</p> $^{35}\text{Cl}^{35}\text{Cl} = 70$ $^{35}\text{Cl}^{37}\text{Cl} = 72$ $^{37}\text{Cl}^{37}\text{Cl} = 74$   | (1)  |
| Question Number | Acceptable Answer  | Additional Guidance   | Mark |
| (iii)           | <ul style="list-style-type: none"> <li>probability of two <math>^{35}\text{Cl}</math> atoms (1)</li> <li>probability of <math>^{35}\text{Cl}</math> and <math>^{37}\text{Cl}</math> atoms (1)</li> <li>probability of two <math>^{37}\text{Cl}</math> atoms (1)</li> </ul> | <p>Example of calculation</p> $\frac{3}{4} \times \frac{3}{4} = \frac{9}{16} = 0.5625$ $2 \times \frac{3}{4} \times \frac{1}{4} = \frac{6}{16} = 2 \times 0.1875 = 0.36995$ $\frac{1}{4} \times \frac{1}{4} = \frac{1}{16} = 0.0625$ <p>(so ratio is 9:6:1)</p> <p>Allow alternative explanations and calculations but the logic must be clear.<br/>e.g. probability tree (3 max)<br/>measurement of peak heights from graph (2 max) eg 3.8:2.4:0.4 = ratio 9:6:1 (approx.)</p> | (1)  |



Q2.

| Question Number                       | Answer   | Additional Guidance   | Mark |       |                         |     |                                       |     |                                       |     |                         |     |     |
|---------------------------------------|--|---|------|-------|-------------------------|-----|---------------------------------------|-----|---------------------------------------|-----|-------------------------|-----|-----|
|                                       | <ul style="list-style-type: none"> <li>all 4 ion formulae<br/>(1)</li> <li>all 4 <math>m/z</math> values<br/>(1)</li> </ul> <p>or</p> <ul style="list-style-type: none"> <li>any two <math>m/z</math> values with corresponding ion formulae<br/>(1)</li> <li>the other two <math>m/z</math> values with corresponding ion formulae<br/>(1)</li> </ul> | <p><u>Example of answer:</u></p> <table> <tr> <td>ions</td> <td><math>m/z</math></td> </tr> <tr> <td><math>P(^{35}\text{Cl})_3^+</math></td> <td>136</td> </tr> <tr> <td><math>P(^{35}\text{Cl})_2^{37}\text{Cl}^+</math></td> <td>138</td> </tr> <tr> <td><math>P^{35}\text{Cl}(^{37}\text{Cl})_2^+</math></td> <td>140</td> </tr> <tr> <td><math>P(^{37}\text{Cl})_3^+</math></td> <td>142</td> </tr> </table> <p>Allow any other unambiguous way of representing the formulae e.g. with brackets or in words</p> <p>Positive charge only needs to be shown on one of the ions</p> <p>Ignore mass number on P</p> | ions | $m/z$ | $P(^{35}\text{Cl})_3^+$ | 136 | $P(^{35}\text{Cl})_2^{37}\text{Cl}^+$ | 138 | $P^{35}\text{Cl}(^{37}\text{Cl})_2^+$ | 140 | $P(^{37}\text{Cl})_3^+$ | 142 | (2) |
| ions                                  | $m/z$  |   |      |       |                         |     |                                       |     |                                       |     |                         |     |     |
| $P(^{35}\text{Cl})_3^+$               | 136  |   |      |       |                         |     |                                       |     |                                       |     |                         |     |     |
| $P(^{35}\text{Cl})_2^{37}\text{Cl}^+$ | 138  |   |      |       |                         |     |                                       |     |                                       |     |                         |     |     |
| $P^{35}\text{Cl}(^{37}\text{Cl})_2^+$ | 140  |   |      |       |                         |     |                                       |     |                                       |     |                         |     |     |
| $P(^{37}\text{Cl})_3^+$               | 142  |   |      |       |                         |     |                                       |     |                                       |     |                         |     |     |

Q3.

| Question Number | Acceptable Answer   | Additional Guidance                                      | Mark |
|-----------------|---|--|------|
| (i)             | <ul style="list-style-type: none"> <li>relative molecular mass</li> </ul> | 170<br>May be shown on graph<br>Do not award peak at 171 | (1)  |

| Question Number | Acceptable Answer   | Additional Guidance   | Mark |
|-----------------|---|---|------|
| (ii)            | <ul style="list-style-type: none"> <li><math>\text{C}_{12}\text{H}_{26}</math></li> </ul> | Allow TE from (i) provided H/C could exist eg DNA 57 = $\text{C}_4\text{H}_9$<br>Allow $\text{C}_{13}\text{H}_{14}$ | (1)  |



Q4.

| Question Number | Acceptable Answers                                     | Additional Guidance  | Mark |
|-----------------|--|--|------|
| (i)             | (identify the peak at the) highest/largest $m/z$ value | Allow<br>Peak (furthest) to the right/last peak on the spectrum<br><br>Do not award the mark for "largest peak" / "highest peak"<br><br>Ignore<br>"parent ion" / molecular ion peak / References to $m/z = 86$ | (1)  |

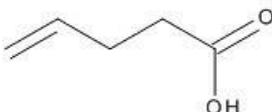
| Question Number | Acceptable Answers   | Additional Guidance  | Mark |
|-----------------|--|--|------|
| (ii)            | $\begin{array}{c} \text{H} & \text{H} & \text{H} \\   &   &   \\ \text{H}-\text{C}-\text{C}^+-\text{C}-\text{H} \\   & &   \\ \text{H} & & \text{H} \end{array}$ <p style="text-align: center;">(1)</p> $\begin{array}{c} \text{H} & \text{O} \\   &    \\ \text{H}-\text{C}-\text{C}^+ \\   \\ \text{H} \end{array}$ <p style="text-align: center;">(1)</p> | Allow positive charge anywhere on structure<br><br>Ignore open bonds<br><br>Penalise non-displayed formulae once only<br><br>Ignore brackets around the structure<br><br>Penalise missing charge once only | (2)  |

Q5.

| Question number | Answer   | Mark |
|-----------------|--|------|
| (i)             | <b>The only correct answer is D</b> ( $\text{C}_5\text{H}_8\text{O}_2$ )<br><i>A is incorrect because <math>\text{C}_7\text{H}_{16}</math> has a molecular ion <math>m/z = 100.1248</math></i><br><i>B is incorrect because <math>\text{C}_6\text{H}_{12}\text{O}</math> has a molecular ion <math>m/z = 100.0885</math></i><br><i>C is incorrect because <math>\text{C}_6\text{H}_{14}\text{N}</math> has a molecular ion <math>m/z = 100.1123</math></i> | (1)  |

| Question Number | Answer   | Additional Guidance  | Mark |
|-----------------|--|--|------|
| (ii)            | <ul style="list-style-type: none"> <li>• alkene / C=C<br/>(1)</li> <li>• carboxylic acid / COOH<br/>(1)</li> </ul> | The functional groups can be in any order<br>Ignore just 'double bond'<br><br>Ignore just C=O and OH | (2)  |



| Question Number | Answer  | Additional Guidance  | Mark |
|-----------------|---|--|------|
| (iii)           | <ul style="list-style-type: none"> <li>skeletal formula of X</li> </ul> | <p>Example of skeletal formula</p>  <p>Ignore bond lengths and bond angles</p> | (1)  |

Q6.

| Question Number | Answer   | Additional Guidance   | Mark |
|-----------------|--|---|------|
| (i)             | <p>An answer that makes reference to the following points:</p> <ul style="list-style-type: none"> <li>chlorine / Cl<sub>2</sub> <b>and</b> ultraviolet / uv (light)</li> </ul> | <p>Allow sunlight<br/>Ignore chlorine radicals<br/>Ignore temperatures<br/>Do not award presence of an additional catalyst<br/>Do not award hydrogen chloride / HCl / hydrochloric acid / HCl(aq)</p> | (1)  |

| Question Number | Answer  | Mark |
|-----------------|---|------|
| (ii)            | <p>The only correct answer is <b>C</b> (free radical substitution)</p> <p><i>A is not correct because as ethane is saturated the reaction is a substitution</i></p> <p><i>B is not correct because as ethane is saturated the reaction is a substitution</i></p> <p><i>D is not correct because as ethane has no bonds with significant polarity the reaction is not nucleophilic</i></p> | (1)  |



| Question Number | Answer  | Additional Guidance  | Mark |
|-----------------|---|--|------|
| (iii)           | <ul style="list-style-type: none"> <li>chloroethane reacts with a chlorine radical</li> </ul> OR<br><br>both correct structure formulae of the products <b>including</b> identification of which is which (1) | Allow radical dots anywhere on the radical species throughout<br><br>$\text{CH}_3\text{CH}_2\text{Cl} + \text{Cl}\cdot \rightarrow \cdot\text{CH}_2\text{CH}_2\text{Cl} + \text{HCl}$<br>or<br>$\text{CH}_3\text{CH}_2\text{Cl} + \text{Cl}\cdot \rightarrow \text{CH}_3\text{CHCl}\cdot + \text{HCl}$<br>Allow<br>$\text{C}_2\text{H}_5\text{Cl} + \text{Cl}\cdot \rightarrow \text{C}_2\text{H}_4\text{Cl}\cdot + \text{HCl}$<br><br>$\text{CH}_3\text{CHCl}_2$ 1,1-dichloroethane<br>$\text{CH}_2\text{ClCH}_2\text{Cl}$ 1,2-dichloroethane | (3)  |
|                 | <ul style="list-style-type: none"> <li>formation of 1,1-dichloroethane via radical mechanism</li> </ul> OR  | $\text{CH}_3\text{CHCl}\cdot + \text{Cl}\cdot \rightarrow \text{CH}_3\text{CHCl}_2$<br>or<br>$\text{CH}_3\text{CHCl}\cdot + \text{Cl}_2 \rightarrow \text{CH}_3\text{CHCl}_2 + \text{Cl}\cdot$<br>Ignore reactions of $\text{C}_2\text{H}_4\text{Cl}\cdot$   |      |

|  |  |  |  |
|--|--|--|--|
|  | overall equation for the formation of 1,1-dichloroethane (1)   | $\text{CH}_3\text{CH}_2\text{Cl} + \text{Cl}_2 \rightarrow \text{CH}_3\text{CH}_2\text{Cl}_2 + \text{HCl}$   |  |
|  | <ul style="list-style-type: none"> <li>formation of 1,2-dichloroethane via radical mechanism</li> </ul> OR<br><br>equation for the formation of 1,2-dichloroethane (1) | $\cdot\text{CH}_2\text{CH}_2\text{Cl} + \text{Cl}\cdot \rightarrow \text{CH}_2\text{ClCH}_2\text{Cl}$<br>or<br>$\cdot\text{CH}_2\text{CH}_2\text{Cl} + \text{Cl}_2 \rightarrow \text{CH}_2\text{ClCH}_2\text{Cl} + \text{Cl}\cdot$<br>Ignore reactions of $\text{C}_2\text{H}_4\text{Cl}\cdot$<br><br>$\text{CH}_3\text{CH}_2\text{Cl} + \text{Cl}_2 \rightarrow \text{CH}_2\text{ClCH}_2\text{Cl} + \text{HCl}$<br><br>If M2 and M3 are not scored allow (1) for a balanced equation for the reaction of $\text{C}_2\text{H}_4\text{Cl}\cdot$ with $\text{Cl}\cdot$ or $\text{Cl}_2$ to form $\text{C}_2\text{H}_4\text{Cl}_2$ (examples shown)<br>$\text{C}_2\text{H}_4\text{Cl}\cdot + \text{Cl}\cdot \rightarrow \text{C}_2\text{H}_4\text{Cl}_2$<br>or<br>$\text{C}_2\text{H}_4\text{Cl}\cdot + \text{Cl}_2 \rightarrow \text{C}_2\text{H}_4\text{Cl}_2 + \text{Cl}\cdot$ |  |



| Question Number | Answer  | Additional Guidance  | Mark |
|-----------------|---|--|------|
| (iv)            | <p>An answer that makes reference to the following points:</p> <ul style="list-style-type: none"> <li>98 peak is due to <math>C_2H_4^{35}Cl_2^+</math></li> <li><b>and</b></li> <li>102 peak is due to <math>C_2H_4^{37}Cl_2^+</math></li> </ul> <p>(1)</p> <ul style="list-style-type: none"> <li>100 peak is due to <math>C_2H_4^{35}Cl^{37}Cl^+</math></li> </ul> <p>(1)</p> | <p>Allow <math>C_2H_4^{35}Cl^{35}Cl^+</math></p> <p>Allow <math>C_2H_4^{37}Cl^{37}Cl^+</math></p> <p>Allow structural formulae of the molecular ions of either 1,1- or 1,2-dichloroethane or both</p> <p>Allow structures with the positive charge anywhere including outside of brackets of any type.</p> <p>Penalise omission of + once only</p> | (2)  |

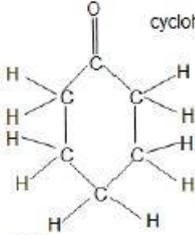
| Question Number | Answer  | Additional Guidance   | Mark |
|-----------------|---|---|------|
| (v)             | <p>An answer that makes reference to the following point</p> <ul style="list-style-type: none"> <li><math>^{35}Cl</math> and <math>^{37}Cl</math> atoms are in a 3:1 ratio</li> </ul> | <p>Answer must refer to the isotopes of chlorine. Ignore comments about isotopes of carbon or hydrogen or just isotopes</p> <p>Allow a larger proportion of chlorine atoms are chlorine-35 than chlorine-37</p> <p>Allow the ratio of the peak heights to be 9:6:1</p> <p>Allow the abundance of chlorine- 35 and chlorine-37 are different</p> <p>Allow there are two isotopes of chlorine</p> | (1)  |



| Question Number | Answer   | Additional Guidance   | Mark |
|-----------------|--|---|------|
| (vi)            | <p>An answer that makes reference to the following points:</p> <p>Either</p> <ul style="list-style-type: none"> <li>the peaks are formed by fragments containing both chlorine atoms attached to one carbon atom</li> </ul> <p>or</p> <p>the fragments are <math>\text{CH}^{35}\text{Cl}^{37}\text{Cl}^+</math>, <math>\text{CH}^{35}\text{Cl}_2^+</math> and <math>\text{CH}^{37}\text{Cl}_2^+</math> (1)</p> <ul style="list-style-type: none"> <li>this fragmentation / configuration is only possible from 1,1-dichloroethane / is not possible from 1,2-dichloroethane (1)</li> </ul> <p>Or</p> <ul style="list-style-type: none"> <li>the peaks at 83, 85 and 87 represent the loss of a <math>\text{CH}_3</math> group (1)</li> <li>only 1,1-dichloroethane has a methyl group (1)</li> </ul> | <p>Allow a diagram showing the fragmentation of 1,1-dichloromethane to form a fragment containing one carbon and two chlorine atoms</p> <p>Allow the use of molecule instead of fragment</p> <p>Do not award fragments where the number of hydrogens on the carbon changes</p> <p>Allow just <math>\text{CHCl}_2^+</math></p> <p>Do not penalise the absence of the positive charge</p> <p>Do not award fragments where the number of hydrogens changes to allow for the different masses</p> <p>Allow only 1,1-dichloroethane has two chlorines on the same carbon / 1,2-dichloroethane does not have two chlorines on the same carbon</p> <p>Allow the peaks are 15 below the molecular ion values so they represent the loss of a <math>\text{CH}_3</math> group</p> | (2)  |



Q7.

| Question Number | Answer   | Additional Guidance  | Mark |
|-----------------|--|--|------|
| (i)             | <p>An answer that makes reference to the following points:</p> <ul style="list-style-type: none"> <li>name (1)</li> <li>displayed formula (1)</li> </ul> | <p><u>Example of displayed formula</u></p>  <p style="text-align: right;">cyclohexanone</p> <p>Allow CH<sub>2</sub> groups<br/>Allow skeletal formula<br/>Do not award molecular formula</p> | (2)  |

| Question Number | Answer   | Additional Guidance  | Mark |
|-----------------|--|--|------|
| (ii)            | <p>An answer that makes reference to the following points:</p> <ul style="list-style-type: none"> <li>O-H bond (stretching) 3750 – 3200 cm<sup>-1</sup> in cyclohexanol is not present in cyclohexanone /disappears (when cyclohexanol reacts). (1)</li> <li>C=O bond (stretching) 1720 – 1700 cm<sup>-1</sup> appears in cyclohexanone (1)</li> </ul> | <p>Allow a range within the specified range</p> <p>Allow 1725 – 1700 cm<sup>-1</sup><br/>Do not allow 1740 – 1720 cm<sup>-1</sup> (aldehyde)</p> | (2)  |

| Question Number | Answer  | Additional Guidance   | Mark |
|-----------------|---|---|------|
| (iii)           | <ul style="list-style-type: none"> <li>highest <math>m/z = M_r = 98</math></li> </ul> | <p>Check, answer may be shown on mass spectrum<br/>Do not accept just '98' with no supporting evidence</p> <p>Allow peak furthest to the right / molecular ion peak is 98</p> | (1)  |



| Question Number | Answer   | Additional Guidance   | Mark |
|-----------------|--|---|------|
| (iv)            | <ul style="list-style-type: none"> <li>fragment (1)</li> <li>charge (1)</li> </ul> | <p>Examples of fragment structure</p> <div style="text-align: center;"> <math display="block">  \begin{array}{c}  \text{CH}^+ \\  \diagdown \quad \diagup \\  \text{CH}_2 \quad \text{CH}_2 \\  \diagup \quad \diagdown \\  \text{CH}_2 \quad \text{CH}_2 \\  \diagdown \quad \diagup \\  \text{CH}_2  \end{array}  </math> </div> <p style="text-align: right;"><math>\text{C}_6\text{H}_{11}^+</math></p> <p>Allow charge anywhere on fragment, including outside brackets around the fragment</p> <p>Allow straight chain fragment provided it has the correct number of C and H atoms</p> | (2)  |

Q8.

| Question Number | Acceptable Answer | Additional Guidance  | Mark |
|-----------------|-------------------|--|------|
| (a)             |                   | display all three methyl groups<br>allow -OH<br>do not award C-H-O | (1)  |

| Question Number | Acceptable Answer  | Additional Guidance | Mark |
|-----------------|--|---------------------|------|
| (b)(i)          | An answer that makes reference to one of the following:<br><br>molecular ion/molecule<br>fragments/is unstable |                     | (1)  |

| Question Number | Acceptable Answer | Additional Guidance  | Mark |
|-----------------|-------------------|--|------|
| (ii)            |                   | allow + charge on any part of the ion/outside the structure but + must be shown<br><br>allow displayed/structural/skeletal/molecular formulae or any combination of these. | (1)  |



| Question Number | Acceptable Answer   | Additional Guidance   | Mark       |
|-----------------|---|---|------------|
| (c)(i)          | <ul style="list-style-type: none"> <li>calculation for bonds broken in the alcohol (*)<br/><b>(1)</b></li> <li>calculation for bonds broken in oxygen<br/><b>(1)</b></li> </ul> <p><b>and</b></p> <p>total energy for bonds broken(**)<br/><b>(1)</b></p> <ul style="list-style-type: none"> <li>calculation for bonds made(***)<br/><b>(1)</b></li> <li>calculation of <math>\Delta_c H</math> (2-methylpropan-2-ol) with sign<br/><b>(1)</b></li> </ul> | <p><u>Example of calculation</u></p> $3(\text{C-C}) + 9(\text{C-H}) + (\text{C-O}) + (\text{O-H})$ $= (3 \times 347) + (9 \times 413) + 358 + 464 = (+)5580 \text{ (kJ mol}^{-1}\text{)}$ $6(\text{O=O}) = (6 \times 498) = (+)2988 \text{ (kJ mol}^{-1}\text{)}$ <p>total = + 5580 + 2988 = (+)8568 (kJ mol<sup>-1</sup>)<br/>TE from ans * M1 + 2988</p> $= 8(\text{C=O}) + 10(\text{O-H})$ $= (8 \times 805) + (10 \times 464) = -11080 \text{ (kJ mol}^{-1}\text{)}$ $= +8568 - 11080 = -2512 \text{ (kJ mol}^{-1}\text{)}$ <p>allow TE for answer(**) + answer(***)<br/>units not required but if given they must be correct<br/>correct final answer with no working scores 4 marks</p> | <b>(4)</b> |

| Question Number | Acceptable Answer  | Additional Guidance   | Mark       |
|-----------------|--|---|------------|
| (ii)            | <p>An explanation that makes reference to the following points:</p> <ul style="list-style-type: none"> <li>incomplete combustion<br/><b>(1)</b></li> <li><math>\Delta_c H</math> (2-methylpropan-2-ol) will be less negative /less exothermic than data book value<br/><b>(1)</b></li> </ul> | <p>mark independently</p> <p>do not award just lower/smaller/decreases/ more positive<br/>allow reduce the magnitude (of the value)</p> | <b>(2)</b> |



| Question Number | Acceptable Answer   | Additional Guidance  | Mark |
|-----------------|---|--|------|
| (iii)           | An answer that makes reference to the following points:<br><br>$\Delta_c H$ figures are at 298 K /data book bond energies refer to gaseous state<br><u>and</u><br>water and/or 2-methylpropan-2-ol are/is (both) liquid(s) (at 298 K) | allow just liquid involved<br><br>do not award data book bond energies are mean (values)/not specific to 2-methylpropan-2-ol | (1)  |

Q9.

| Question Number | Acceptable Answers  | Additional Guidance  | Mark |
|-----------------|---|--|------|
| (a)             | <ul style="list-style-type: none"> <li>calculation of empirical formula (1)</li> <li>uses molecular ion to prove molecular formula (1)</li> </ul> <p>or</p> <ul style="list-style-type: none"> <li>calculation of percentage of each element in compound<br/>all 3 correct scores (2)<br/>any 2 correct scores (1)</li> </ul> <p>or</p> <ul style="list-style-type: none"> <li>calculation of the number of atoms of each element directly<br/>all 3 correct scores (2)<br/>any 2 correct scores (1)</li> </ul> | <p>Example of calculation</p> $\begin{array}{r} \text{C} : \text{H} : \text{O} \\ \hline 68.2 \quad 13.6 \quad 18.2 \\ 12 \quad 1 \quad 16 \\ = \quad 5.68 \quad 13.6 \quad 1.14 \\ = \quad 5 \quad 12 \quad 1 \end{array}$ <p>Use of 88 to show molecular formula is <math>\text{C}_5\text{H}_{12}\text{O}</math><br/>e.g. <math>M_r</math> is <math>(5 \times 12) + (12 \times 1) + 16 = 88</math> or states that <math>M_r</math> of empirical formula is 88</p> <p>or</p> $\% \text{C} = \frac{5 \times 12 \times 100}{88} = 68.2$ $\% \text{H} = \frac{12 \times 1 \times 100}{88} = 13.6$ $\% \text{O} = \frac{1 \times 16 \times 100}{88} = 18.2$ <p>or</p> $\text{C atoms} = \frac{68.2 \times 88}{100 \times 12} = 5$ $\text{H atoms} = \frac{13.6 \times 88}{100 \times 1} = 12$ $\text{O atoms} = \frac{18.2 \times 88}{100 \times 16} = 1$ | (2)  |
| Question Number | Acceptable Answers  | Additional Guidance  | Mark |
| (b)(i)          | <ul style="list-style-type: none"> <li>(X is a) primary/ 1° (alcohol)</li> </ul>  |  | (1)  |

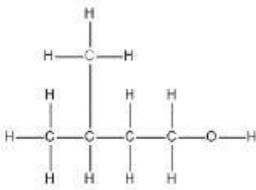


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|-----------------|--------------------|---|------|
| (b)(ii)         |                    | <p>Allow alcohols in any order</p> <p>Allow CH<sub>3</sub> / OH</p> <p>Allow slip of 1 H missing from 1 alcohol / 1 C-C bond missing</p> <p>Ignore names, even if incorrect</p> <p>Penalise O-H-C- / -C-H-O at end of molecule once only</p> <p>If no other mark is given, allow (2) for 4 correct skeletal / structural formulae or any combination of these or (1) for 3 correct</p> <p>Allow (2) for displayed formulae of pentan-2-ol, pentan-3-ol and 3-methylbutan-2-ol if secondary alcohol in (b)(i), or (1) for any two of those</p> | (3)  |

|   |                                  |   |  |
|---|----------------------------------|---|--|
| <ul style="list-style-type: none"> <li>• 4 correct</li> <li>• 3 correct</li> <li>• 2 correct</li> </ul> | <p>(3)</p> <p>(2)</p> <p>(1)</p> | <p>If no other mark awarded and if (b)(i) is blank or incorrect, allow (2) for any 4 different alcohols with formula C<sub>5</sub>H<sub>12</sub>O, (1) for 3 alcohols</p> |  |
|---|----------------------------------|---|--|

| Question Number | Acceptable Answers                                   | Additional Guidance  | Mark |
|-----------------|--|--|------|
| (b)(iii)        | <ul style="list-style-type: none"> <li>• </li> </ul> | <p>Allow structural formula or any combination of displayed and structural formula</p> <p>Allow + anywhere on structure or outside of a formula in a bracket</p> <p>Do not allow C<sub>2</sub>H<sub>5</sub>O<sup>+</sup>/C<sub>2</sub>H<sub>4</sub>OH<sup>+</sup></p> <p>Do not allow missing charge</p> <p>Allow CH<sub>3</sub>C<sup>+</sup>HOH if secondary alcohol identified in (b)(i)</p> | (1)  |



| Question Number | Acceptable Answers   | Additional Guidance  | Mark |
|-----------------|--|--|------|
| (b)(iv)         | <ul style="list-style-type: none"> <li>  </li> </ul> <p>(1)</p> <ul style="list-style-type: none"> <li>because this is the <b>only</b> alcohol with a branched chain <u>and</u> forms <math>\text{CH}_2\text{OHCH}_2^+</math> / <math>\text{C}_2\text{H}_4\text{OH}^+</math> / peak at 45 / fragment identified in (b)(iii)</li> </ul> <p>(1)</p> | <p>Allow any type of identification, including name 3-methylbutan-1-ol</p> <p>Ignore incorrect name with correct structure</p> <p>Conditional on correct identification<br/>Ignore missing charge on fragment</p> <p>Allow reasons why the others are not correct e.g. not pentan-1-ol as it is not branched <u>and</u> not 2-methylbutan-1-ol or 2,2-dimethylpropan-1-ol as they do not form <math>\text{CH}_2\text{OHCH}_2^+</math></p> <p>If secondary alcohol identified in (b)(i):<br/>Allow 3-methylbutan-2-ol (1) as it is the only alcohol with a branched chain that forms <math>\text{CH}_3\text{C}^+\text{HOH}</math> (1)</p> | (2)  |

## Q10.

| Question Number | Acceptable Answer                           | Additional Guidance   | Mark |
|-----------------|---|---|------|
| (i)             | furthest peak to right/ highest $m/z = 154$ | <p>Ignore just 'highest peak'</p> <p>may be shown on spectrum alone provided 154 stated</p> <p>Allow parent ion/molecular ion/last peak at 154</p> <p>Must see the figure 154 in text or on graph</p> | (1)  |

| Question Number | Acceptable Answer                                     | Additional Guidance   | Mark |
|-----------------|---|---|------|
| (ii)            | $\text{C}_5\text{H}_9^+$ / $[\text{C}_5\text{H}_9]^+$ | <p>+ charge is essential, allow charge anywhere on the ion/ outside / inside brackets</p> <p>Allow displayed/structural/skeletal formula or any combination of these.</p> <p>Ignore name of ion even if incorrect<br/>(Correct name: 2-methylbut-2-ene ion)</p> | (1)  |



Q11.

| Question Number | Acceptable Answers  | Additional Guidance  | Mark       |
|-----------------|---|--|------------|
|                 | <ul style="list-style-type: none"> <li>molecular ion is at <math>m/z = 168</math><br/><b>or</b><br/>168 is equal to the <math>M_r</math> of <b>D</b> /<br/>twice the empirical formula /<br/><math>2 \times 84 / 168 \div 2 = 84 /</math><br/><math>M_r</math> of empirical formula is 84 <b>(1)</b></li> <li>(so the molecular formula is) <math>C_6H_4N_2O_4</math> <b>(1)</b></li> </ul> | <p>Allow 168 shown on spectrum along with the rest of the explanation<br/>Do not award M1 for any other value</p> <p>Stand alone mark<br/>Ignore structural / displayed / skeletal formula</p> <p>Do not award <math>C_6H_4N_2O_4^+</math></p> | <b>(2)</b> |

Q12.

| Question Number | Answer  | Additional Guidance   | Mark       |
|-----------------|---|---|------------|
| (i)             | <ul style="list-style-type: none"> <li>calculate percentage of carbon <b>(1)</b></li> <li>division of all percentages by atomic mass <b>(1)</b></li> <li>find simplest ratio and give empirical formula <b>(1)</b></li> </ul> | <p>Example of calculation:</p> <p><math>100 - (34.0 + 54.5) = 11.5\%</math></p> <p>Cl <math>34.0 / 35.5 = 0.95775</math><br/>F <math>54.5 / 19.0 = 2.8684</math><br/>C <math>11.5 / 12.0 = 0.95833</math></p> <p>Cl <math>(0.95775 / 0.95775 = 2.9949) = 1</math><br/>F <math>(2.8684 / 0.95775 = 2.9949) = 3</math><br/>C <math>(0.95833 / 0.95775 = 2.9949) = 1</math></p> <p>So <math>CF_3Cl</math> / <math>CClF_3</math></p> <p>Allow any order</p> <p>Correct answer with no working scores (3)<br/>Ignore significant figures throughout.</p> | <b>(3)</b> |



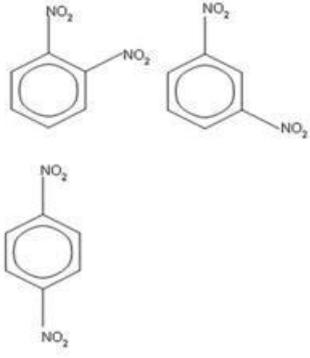
| Question Number | Answer   | Additional Guidance   | Mark |
|-----------------|--|---|------|
| (ii)            | <p>An answer that makes reference to the following points:</p> <ul style="list-style-type: none"> <li>molecular ion peak at 104 / 106 (which matches the mass of the empirical formula)</li> </ul> | Do not award statements stating that the molecular ion peak is at 105 or at 104.5, unless this is a calculated average. | (1)  |

| Question Number | Answer  | Additional Guidance   | Mark |
|-----------------|---|---|------|
| (iii)           | <ul style="list-style-type: none"> <li>correct ion</li> </ul> | $\text{CF}_3^+$<br>Do not award $\text{CF}_3$ with no plus. | (1)  |

Q13.

| Question Number | Acceptable Answers       | Additional Guidance  | Mark |
|-----------------|--------------------------|--|------|
| (i)             | $\text{C}_6\text{H}_4^+$ | Allow $\text{H}_4\text{C}_6^+$<br><br>Do not award just $\text{C}_6\text{H}_4$ | (1)  |



| Question Number | Acceptable Answers   | Additional Guidance   | Mark |
|-----------------|--|---|------|
| (ii)            | <ul style="list-style-type: none"> <li>3 correct formulae (2)</li> </ul> | <p><u>Examples of formulae</u></p>  <p>Allow (1) for any 2 correct formulae</p> <p>Allow (2) for three disubstituted benzenes with incorrect substituents / (1) for any two disubstituted benzenes with incorrect substituents</p> <p>Allow incorrectly displayed formulae of NO<sub>2</sub> groups</p> <p><b>In (c)(ii) and (iii):</b><br/>           Allow Kekule structures<br/>           Allow hydrogen atoms shown on benzene<br/>           Ignore connectivity of NO<sub>2</sub> groups<br/>           Penalise missing circle in benzene once only</p> | (2)  |



| Question Number | Acceptable Answers   | Additional Guidance  | Mark       |
|-----------------|--|--|------------|
| (iii)           | <ul style="list-style-type: none"> <li>• <b>D</b> identified as 1,3-dinitrobenzene <b>and</b> 4 different carbon environments labelled <b>(1)</b></li> <li>• 3 different carbon environments labelled on 1,2-dinitrobenzene <b>(1)</b></li> <li>• 2 different carbon environments labelled on 1,4-dinitrobenzene <b>(1)</b></li> </ul> | <div style="text-align: center;"> </div> <p><u>Examples of identification</u></p> <p>These labels may be shown on the structures in (c)(ii)</p> <p>The identification of <b>D</b> can be assumed if it is the only structure with 4 carbon environments labelled</p> <p>Allow any form of identification of the carbon environments e.g. numbers, letters, equivalent carbon environments circled</p> <p>TE on disubstituted benzene substituents in (ii)</p> <p>Penalise only half the carbon environments labelled once only</p> | <b>(3)</b> |