

# Spectroscopy (IR & Mass Spec)

## Mark Scheme

Level	International A Level
Subject	Chemistry
Exam Board	Edexcel
Topic	Chemistry Lab Skills 1
Sub Topic	Spectroscopy (IR & Mass Spec)
Booklet	Mark Scheme

**Time Allowed:** 41 minutes

**Score:** /34

**Percentage:** /100

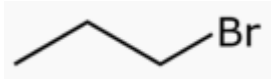
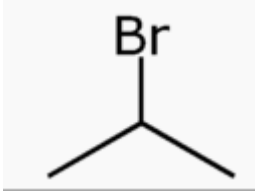
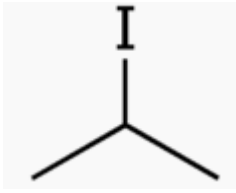
**Grade Boundaries:**

A*	A	B	C	D	E	U
>85%	'77.5%	70%	62.5%	57.5%	45%	<45%

Question Number	Acceptable Answers	Reject	Mark
<b>1(a)</b>	<p>Ethanol dissolves (both) halogenoalkanes (and silver nitrate)</p> <p>To allow the halogenoalkane and water/silver nitrate to mix</p> <p>To allow reactants to mix</p> <p>OR</p> <p>Ethanol is a <b>co-solvent</b></p> <p>ALLOW</p> <p>Ethanol has polar and non-polar parts/is a polar and non-polar solvent/ dissolves ionic and covalent substances</p> <p>IGNORE</p> <p>Halogenoalkanes are insoluble in water</p>	<p>Just 'to provide the same reaction conditions'</p> <p>Just 'ethanol is a solvent'</p>	1

Question Number	Acceptable Answers	Reject	Mark
<b>1(b)</b>	<p><b>P and Q</b> bromine/Br/C<sub>3</sub>H<sub>7</sub>Br/bromoalkane</p> <p>ALLOW AgBr <b>(1)</b></p> <p><b>R</b> iodine/I/C<sub>3</sub>H<sub>7</sub>I/bromoalkane</p> <p>ALLOW AgI <b>(1)</b></p> <p>Penalise halide ion(s) only once</p> <p>Penalise X<sub>2</sub> only once</p>	Bromine <b>and</b> chlorine	2

Question Number	Acceptable Answers	Reject	Mark
<b>1(c)(i)</b>	<p>CH<sub>3</sub>CH<sub>2</sub><sup>+</sup> / C<sub>2</sub>H<sub>5</sub><sup>+</sup></p> <p>ALLOW</p> <p>Structural, displayed, skeletal formulae.</p> <p>Allow charge anywhere on fragment, including outside brackets.</p>	<p>Absence of charge</p> <p>/ C<sub>2</sub>H<sub>5</sub><sup>-</sup></p> <p>/ C<sub>2</sub>H<sub>5</sub>-</p> <p><b>ethane</b> ion</p>	1

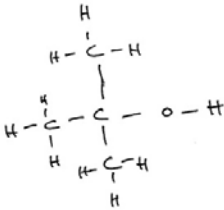
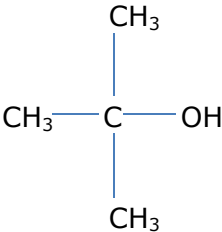
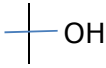
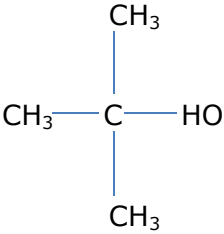
Question Number	Acceptable Answers	Reject	Mark
<b>1(c)(ii)</b>	<p><b>P</b> <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}</math> (1)</p> <p><b>Q</b> <math>\text{CH}_3\text{CHBrCH}_3</math> (1)</p> <p><b>R</b> <math>\text{CH}_3\text{CHICH}_3</math> (1)</p> <p>ALLOW</p> <p>Displayed or skeletal formulae for any or all parts</p> <p><b>P</b> </p> <p><b>Q</b> </p> <p><b>R</b> </p> <p>TE for incorrect halogen(s) in 2(b)</p> <p>Penalise the same error in structural/displayed/skeletal formulae once only.</p> <p><b>Special cases</b></p> <p><b>P</b> <math>\text{CH}_3\text{CHBrCH}_3</math>, <b>Q</b> <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}</math>, and <b>R</b> <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{I}</math> (1)</p> <p><b>P</b> <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}</math>, <b>Q</b> <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}</math>, and <b>R</b> <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{I}</math> (1)</p>		3

(Total for Question 1 = 7 marks)

Question Number	Acceptable Answers	Reject	Mark
2(a)	<p><b>ST</b> Add <math>\text{PCl}_5</math> / phosphorus(V) chloride / phosphorus pentachloride / <math>\text{SOCl}_2</math> / thionyl chloride / sulphur dichloride oxide (1)</p> <p><b>RESULT</b> Mark depends on correct reagent, but allow <math>\text{PCl}_5</math> (aq)</p> <p>Steamy / misty / white fumes ALLOW Gas for fumes (1)</p> <p>Ignore incorrect identification of fumes</p> <p><b>OR</b></p> <p><b>TEST</b> Add sodium / Na (1)</p> <p><b>RESULT</b> Mark depends on correct reagent</p> <p>Effervescence / bubbling / fizzing</p> <p>Ignore incorrect identification of fumes and tests for products</p> <p>white solid (forms) / sodium dissolves</p> <p>mixture gets hot (1)</p>	<p>Acidified <math>\text{PCl}_5</math> / <math>\text{PCl}_5</math> (aq)</p> <p>Acidified dichromate(VI) <math>\text{PCl}_3</math></p> <p>Test to form an ester</p> <p>Any smoke Just "HCl fumes" Just "gas turns litmus red"</p> <p>Just "hydrogen"</p>	2

Question Number	Acceptable Answers	Reject	Mark
2(b)	(primary / secondary / tertiary) Alcohol <b>and</b> carboxylic acid  ALLOW ROH <b>and</b> RCOOH R <sub>2</sub> CHOH/ R <sub>3</sub> COH for ROH C <sub>n</sub> H <sub>2n+1</sub> OH for ROH RCO <sub>2</sub> H for RCOOH Phenol(s) (as one alternative) Fatty acid / alkanolic acid for carboxylic acid	diol carboxyl cyclic alcohol specific alcohol eg ethanol	1

Question Number	Acceptable Answers	Reject	Mark
2(c)	Z identified as tertiary alcohol (1)  <b>Justification:</b> Any one from  Test with litmus Not (carboxylic) acid because there is no change (in (blue) litmus paper)  It's an alcohol because there is no change (in (red / blue) litmus paper)  It is neutral /not an acid or an alkali because there is no change (in (red / blue) litmus paper)  Test with dichromate It is a tertiary alcohol because it can't be oxidized (by acidified dichromate(VI))/ doesn't react with acidified dichromate(VI)  It is not a primary or secondary alcohol because it can't be oxidized (by acidified dichromate(VI))/ doesn't react with acidified dichromate(VI)  IGNORE Not an amine (1)  If more than one justification is given, both must be correct		2

Question Number	Acceptable Answers	Reject	Mark
2(d)	<p>MP1 (0.1 mol Z produces) 0.4 mol CO<sub>2</sub> OR 1 mol Z produces 4 mol CO<sub>2</sub> (1)</p> <p>MP2 (dependent on MP1 awarded) So Z has 4C atoms ALLOW Formula shown with 4C (1)</p> <p>MP3 (stand alone)</p>  <p>OR</p>  <p>ALLOW undisplayed CH<sub>3</sub> and OH as above Skeletal formula</p>  <p>(1)</p>	<p>Just 9.6/24 = 0.4 with no reference to what numbers refer to or if not applied</p>  <p>Only if bond clearly shown to the H of OH</p>	3

Question Number	Acceptable Answers	Reject	Mark
2(e)(i)	<p>Molecular ions have same <math>m/e</math></p> <p>ALLOW</p> <p>same molecular ion isomers have same molar mass / molecular mass molecular ion with same mass same maximum <math>m/e</math> value same peak furthest to right same last peak Parent ion / <math>M^+</math> for molecular ion</p> <p>IGNORE</p> <p>Reference to peak heights</p>	<p>Same fragments Same <math>m/e</math> value for highest peak</p> <p>Similar for "same"</p>	1

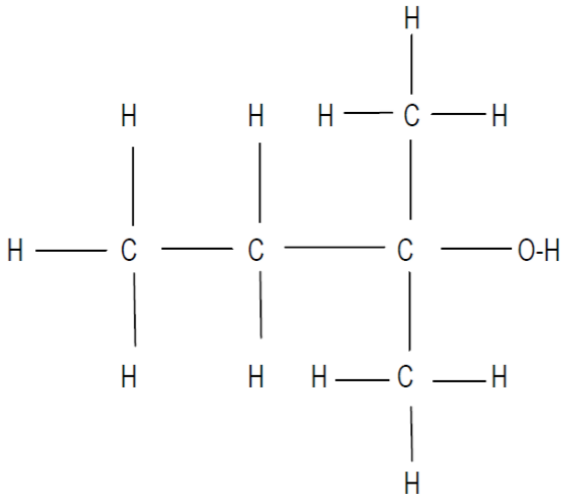
Question Number	Acceptable Answers	Reject	Mark
2(e)(ii)	<p>They both have an (absorption) peak for (wavenumber of) alcohol / hydroxyl group / O-H</p> <p>ALLOW</p> <p>both have peak for -OH / OH frequency / wavelength for wavenumber</p> <p>IGNORE</p> <p>wavenumber values have peak with specific shape for OH</p>	Absorption for C-OH	1

Total for Question 2 = 10 marks

Question Number	Acceptable Answer	Reject	Mark
<b>3(a)(i)</b>	From maximum value of $m/e$ OR From maximum value of $m/z$ OR From maximum mass / charge ratio OR From (position of) peak furthest to right of spectrum (excluding small peaks due to isotopes)  ALLOW Value furthest to the right hand side from (position of) last peak "line" for peak  IGNORE Molecular ion	Just "highest value" Biggest peak Highest peak	<b>1</b>

Question Number	Acceptable Answers	Reject	Mark
<b>3a(ii)</b>	$x = 5$ $y = 11$		<b>1</b>



Question Number	Acceptable Answers	Reject	Mark
<b>3(b)</b>	 <p>TE on (a)(ii) for a correct tertiary alcohol with the number of C atoms given in (a) (ii)</p> <p>ALLOW Partial display eg -OH, -CH<sub>3</sub>, -C<sub>2</sub>H<sub>5</sub></p> <p>ALLOW  <math display="block">\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3\text{-C-OH} \\   \\ \text{C}_2\text{H}_5 \end{array}</math> </p>	<p>Structure shown as fully structural (no bonds shown)</p> <p>skeletal formula</p> <p>-HO Bonds should not go from C to H of OH</p>	<b>1</b>

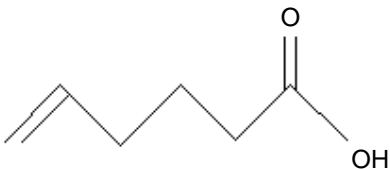
Question Number	Acceptable Answer	Reject	Mark
<b>3(c) (i)</b>	Hydrogen chloride / hydrochloric acid / HCl / HCl(aq)		<b>1</b>

Number			
<b>3(c)(ii)</b>	$\text{NH}_3(\text{g}) + \text{HCl}(\text{g}) \rightarrow \text{NH}_4\text{Cl}(\text{s})$ <p>Correct formulae</p> <p>ALLOW  <math>\text{NH}_4^+ \text{Cl}^- / \text{NH}_4^+ + \text{Cl}^-</math>                      Multiples (1)</p> <p>State symbols (1)</p> <p>Second mark depends on equation showing <b>only</b> correct species even if unbalanced.</p> <p>ALLOW  <math>\text{HCl}(\text{aq})</math></p>		<b>2</b>

Question Number	Acceptable Answer	Reject	Mark
<b>3(d)</b>	<p>Alcohol has a peak for O-H bond                      OR                      ether has no peak for O-H bond</p> <p>ALLOW                      Alcohol has a peak for                      C-OH / C-O-H / -OH</p> <p>OR  <b>Identification from C-O if stated that</b> C-O in ether absorbs at a different wavenumber from C-O in alcohol / ether has C-O-C</p> <p>OR                      Look at fingerprint region <b>and</b> compare with a compound of known identity</p> <p>ALLOW                      Use of "absorption / stretch / vibration / wave number / reading / drop / trough" instead of peak                      R-O for C-O</p> <p>IGNORE "ester" if apparently written by mistake for "ether"                      Broad and sharp (peaks)</p>	<p>Just 'alcohol has an OH bond / group'</p> <p>Just identification from C-O without detail                      C-O peak higher in ether</p> <p>range / spectrum instead of peak</p>	<b>1</b>

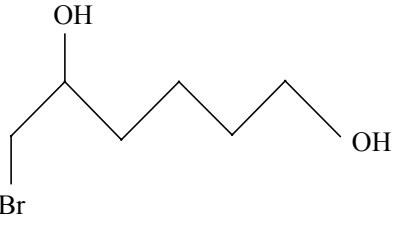
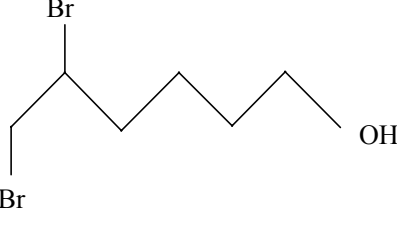
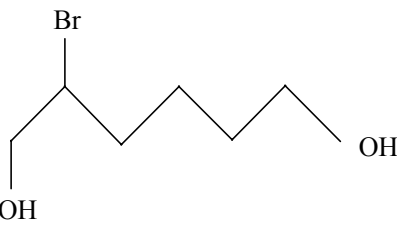
Total for Question 3 = 7 marks

Question Number	Acceptable answers	Reject	Mark
<b>4(a)(i)</b>	Orange to green / blue / brown  ALLOW Dark green / green-brown	Combinations of blue and green Green to orange	<b>1</b>

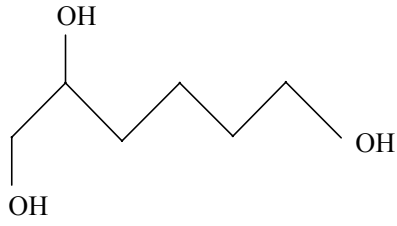
Question Number	Acceptable answers	Reject	Mark
<b>4(a)(ii)</b>	CH <sub>2</sub> =CH(CH <sub>2</sub> ) <sub>3</sub> COOH Double bond need not be shown  ALLOW CO <sub>2</sub> H for COOH  ALLOW   ALLOW displayed formula	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>  Formulae not showing H atoms	<b>1</b>

Question Number	Acceptable answers	Reject	Mark
<b>4(b)</b>	Any TWO of  Bubbles / effervescence / fizzing  Sodium dissolves / disappears  <b>White</b> residue / solid / ALLOW <b>White</b> precipitate  ALLOW Rise in temperature / gets hotter / heat is given out  IGNORE Moves / Floats / Sinks / Catches fire / Hydrogen given off	Just "Gas forms" Bubbles form if incorrect gas identified.  White solid dissolves  Crystals form  Just "exothermic"	<b>2</b>

Question Number	Acceptable answers	Reject	Mark
<b>4(c)(i)</b>	Brown / red-brown / orange / yellow / combinations of these colours to colourless	Red to colourless Clear for colourless Paler for colourless White for colourless	<b>1</b>

Question Number	Acceptable answers	Reject	Mark
<p><b>4(c)(ii)</b></p>	<div style="text-align: center;">  </div> <p>ALLOW</p> <div style="text-align: center;">  </div> <p>ALLOW</p> <div style="text-align: center;">  </div> <p>IGNORE orientation of Br and OH, eg both Br pointing down            IGNORE lengths of bonds</p> <p>Check that there are <b>6C</b> in formula</p>	<p>Br at left hand end without a bond to it</p>	<p><b>1</b></p>

Question Number	Acceptable answers	Reject	Mark
<b>4(d)(i)</b>	Purple / pink to colourless  ALLOW For purple pink: pinkish-purple, dark purple For colourless: brown	Clear for colourless White for colourless Green / orange for colourless Lilac for purple	<b>1</b>

Question Number	Acceptable answers	Reject	Mark
<b>4(d)(ii)</b>	 <p>IGNORE orientation of OH, eg both OH pointing down IGNORE lengths of bonds Check that there are <b>6C</b> in formula</p>	OH at left hand end without a bond to it  Bond to H of OH group	<b>1</b>

Question Number	Acceptable answers	Reject	Mark
<b>4(e)</b>	hex-5-en-1-ol  Alkene/ C=C at 1669 – 1600 (cm <sup>-1</sup> ) (alkene) C-H at 3100-3010 (cm <sup>-1</sup> )  Correct identification <b>and</b> one correct piece of evidence ( <b>1</b> )  Correct identification with two pieces of evidence ( <b>2</b> )  Correct identification and correct bonds quoted without any data can score 1.		<b>2</b>

Total for Question 4 = 10 marks