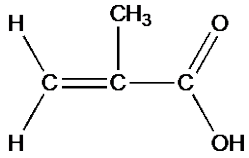
Question number	Answer	Marks	Guidance
1	C : H : O = 55.8/12.0 : 7.0/1.0 : 37.2/16.0 = 4.65 : 7.0 : 2.325 = C_2H_3O Molecular formula = $C_2H_3O \times 86/43 = C_4H_6O_2$ Peak X: $C_3H_5^+$ Peak Y: $COOH^+$ Peak at 1630–1820 cm^{-1} indicates presence of C=O AND peak at 2500–3300 cm^{-1} indicates the presence of –OH group linked carboxylic acid/COOH Structure of **G**  (1 mark available for another carboxylic acid of $C_4H_6O_2$: $H_2C{=}CHCH_2COOH$ or $CH_3CH{=}CHCOOH$)	B1 B1 B1 B1 B1 B2	**ALLOW** mass of C = 0.558 x 86 **or** 48 **AND** mass of H = 0.07 x 86 **or** 6 **AND** mass of O = 0.372 x 86 = 32 + charge required for each response **ALLOW** one mark if both formulae are correct but with no charge/incorrect charge **ALLOW** any possible fragments that contain C, H and/or O that have the correct mass. E.g. Peak X indicates C_2OH^+, Peak **Y** indicates $C_2H_5O^+$ Unfeasible fragments are not allowed e.g. $C_3H_9^+$ (too many H atoms) **LOOK ON THE SPECTRUM** for labelled absorbance which can be given credit Candidates must link absorbance to bond in order to gain the mark **ALLOW** 1700 cm^{-1} For 2500–3300 cm^{-1}, **ALLOW** 2900 cm^{-1} or any stated wavenumber with range 2500–3300 cm^{-1} ALLOW wavenumber range up to 2400–3500 cm^{-1} **ALLOW** structural, skeletal or displayed formula. **DO NOT ALLOW ECF** from incorrect molecular formula
2	C : H : O = 66.7/12.0 : 11.1/1.0 : 22.2/16.0 = 5.56 : 11.1 : 1.39 = C_4H_8O Molecular formula = $C_4H_8O \times 72/72 = C_4H_8O_2$ Peak at 1630–1820 cm^{-1} indicates presence of C=O	B1 B1 B1 B1 x 3	**PLEASE LOOK AT THE SPECTRA AND ABOVE THE SPECTRA FOR POSSIBLE ANSWERS** **ALLOW** two marks for 72 x 66.7/100 = 48/12 = 4 (C) 72 x 11.1/100 = 8 = 8 (H) 72 x 22.2/100 = 16 = 1 (O) **ALLOW** C=O or carbonyl since has absorbance within the range 1640 to 1750 cm^{-1} **ALLOW** ketone **OR** aldehyde linked to correct absorbance

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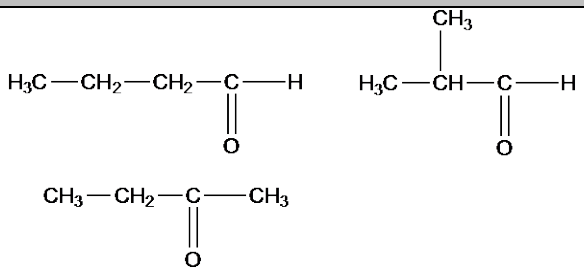
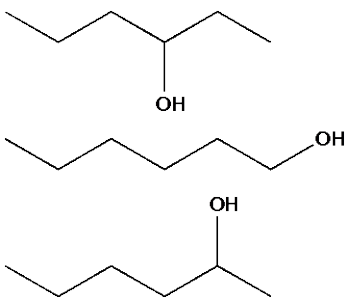
	 1 mark for each structure		**ALLOW** 'could be aldehyde, ketone, carboxylic acid, ester (or amide) because of absorbance between range 1640 to 1750 cm^{-1}' (ie direct quote from the data book) **DO NOT ALLOW** reference to **M** being a carboxylic acid, ester or amide **unless** they are included in a list with aldehyde/ketone in which case **IGNORE** carboxylic acid/ester/amide **IGNORE** reference to C—O / absence of O—H **DO NOT ALLOW** has O—H **ALLOW** correct structural **OR** displayed **OR** skeletal formula **OR** mixture of the above (as long as unambiguous) **eg** $CH_3CH_2CH_2CHO$, $CH_3COCH_2CH_3$ **OR** $(CH_3)_2CHCHO$ **DO NOT ALLOW** C_3H_7CHO **IGNORE** incorrect name correct name on its own is not sufficient
3	C : H : O = 0.600/12.0 : 0.133/1.0 : 0.267/16.0 = 0.0500 : 1.33 : 0.0167 Empirical formula = C_3H_8O Molecular formula = $C_3H_8O \times 60/60 = C_3H_8O$ Peak at 3200–3600 cm^{-1} indicates the presence of –OH group in alcohol **X**: $CH_3CH_2CH_2OH$ OR $CH_3CH(OH)CH_3$ *m/z* at 31 = CH_2OH^+ Links CH_2OH^+ evidence to conclusion that **X** is $CH_3CH_2CH_2OH$	B1 B1 B1 B1 B1 B1 B1	**ALLOW** correct structural **OR** displayed **OR** skeletal formula **OR** mixture of the above (as long as unambiguous) **IGNORE** names **ALLOW** a carboxylic acid reacts with an alcohol to give an ester. **IGNORE** ethanoic acid (as this is stated in the question) **ALLOW** correct structural **OR** displayed **OR** skeletal formula **OR** mixture of the above (as long as unambiguous) If no structure of **X** is provided one mark can be awarded for a correct structure of $CH_3COOCH_2CH_2CH_3$ **OR** $CH_3COOCH(CH_3)_2$ **DO NOT ALLOW** CH_3O^+ **QWC** must link the evidence to

Question number	Answer	Marks	Guidance
			the structure of propan-1-ol. In equation **ALLOW** correct structural **OR** displayed **OR** skeletal formula **OR** mixture of the above
4	C : H : O = 70.59/12.0 : 13.72/1.0 : 15.69/16.0 = 5.8825 : 13.72 : 0.9806 Empirical formula = $C_6H_{14}O$ From mass spectrum, M_r = 102 Molecular formula = $C_6H_{14}O \times 102/102 = C_6H_{14}O$ Peak at 3350 cm^{-1} indicates the presence of –OH group in alcohol  1 mark for each structure	B1 B1 B1 B1 B1 B1 x 3	**ALLOW** two marks for correct empirical formula with no working out **ALLOW** structural or displayed formulae **IGNORE** incorrect names **ALLOW** one minor slip in drawing structures e.g. one missing hydrogen but **ALLOW** ecf for bigger slips such as showing just sticks and no hydrogen atoms **ALLOW** bond to H in OH **ALLOW one** mark for three isomers of $C_6H_{13}OH$ whether branched or unbranched as a catch mark if no other mark has been awarded for the structures If more than three isomers of $C_6H_{13}OH$ drawn • 1 branched and 3 unbranched award **two** marks • any other combination award **one** mark **ALLOW** one mark for hexan-1-ol, hexan-2-ol and hexan-3-ol if structures not drawn
5	Peak at 1630–1820 cm^{-1} indicates presence of C=O Absence of peak at 2500–3300 cm^{-1} indicates the there is no –OH for a carboxylic acid/COOH *m/z* at 60 = molecular ion peak, M^+ *m/z* at 45 = $C_2H_5O^+$ OR loss of CH_3 Links CH_2OH^+ evidence to conclusion that **X** is $CH_3CH_2CH_2OH$ **F**: propanone, CH_3COCH_3	B1 B1 B1 B1 B1	**mass spec of E– Remember to check the spectrum Quality of Written Communication** – mass spec gives M^+ or molecular ion of 60 **OR** mass spec gives parent ion of 60 **OR** highest *m/z* (**ALLOW** *m/e*) value is 60 *m/z* = 45 indicates loss of CH_3 **OR** *m/z* = 45 indicates presence of CH_3CHOH **OR** CH_2CH_2OH **OR** C_2H_5O **IR of F – Remember to check**

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	E: propan-2-ol, $CH_3CH(OH)CH_3$ $CH_3CH(OH)CH_3 + [O] \rightarrow CH_3COCH_3 + H_2O$	B1 B1	**the spectrum** IR shows no broad absorption between 2500 to 3300 cm^{-1} so no O—H bond OR no broad absorption between 2500 to 3300 cm^{-1} so not a carboxylic acid IR shows absorption at 1700 cm^{-1} due to a C=O bond **OR** absorption at 1700 cm^{-1} indicates a ketone **OR** aldehyde present **Identification and equation** **F** is CH_3COCH_3 **OR** propanone **E** is CH3CHOHCH3 **OR** propan-2-ol $CH_3CHOHCH_3 + [O] \longrightarrow CH_3COCH_3 + H_2O$ If **F** has been incorrectly identified as propanal, mark identification and equation as ECF, so max = 2 **ALLOW E** is $CH_3CH_2CH_2OH$ **ALLOW**: $CH_3CH_2CH_2OH + [O] \rightarrow CH_3CH_2CHO + H_2O$
6 (a)	Peak at 2850–3100 cm^{-1} indicates presence of C–H Absence of other characteristic peaks	B1 B1	Answer must have a reference to infrared spectrum i.e. use of cm^{-1} or data from the infrared spectrum 'Has no other peaks so no functional groups present' is **not** sufficient **BUT** There are no peaks due to functional groups is sufficient **ALLOW** peaks instead of absorption **ALLOW** no absorption due to C=O and O–H / no absorption due to carbonyl and hydroxyl
6 (b)	*m/z* at 58 = molecular ion peak, M^+ and evidence of $M(C_4H_{10})$ linked to 58	B1	**ALLOW** peak at *m/z* 58 marked on the mass spectrum / M peak is 58 / peak at 58 linked to the molecular mass **DO NOT ALLOW** highest peak but **ALLOW** 58 is the highest peak

Question number	Answer	Marks	Guidance
6 (c)	*m/z* 15: CH_3^+ *m/z* 29: $C_2H_5^+$ *m/z* 43: $C_3H_7^+$ / $CH_3CH_2CH_2^+$ / $(CH_3)_2CH^+$	B1 B1 B1	Essentially marks are allocated as positive ions Formula of two fragments correct (ignore charge) **BUT** formulae of all three fragments correct (ignore charge)
6 (d)	**A**: $CH_3CH_2CH_3$ linked to peak at *m/z* 29	B1	**ALLOW** name, displayed or skeletal structure **ALLOW** butane because there is a C2H5 fragment **ALLOW** butane because it gives all three fragments listed in **(c)**