

Student 3: Low Merit

NZQA Intended for teacher use only

Mass Spec:

m/z ratio	group
88	C ₂ H ₄ O is the empirical formula and has a mass of 44 so compound must have formula C ₄ H ₈ O ₂ . This is the molecular ion peak.
45	COOH
29	C ₂ H ₅

IR:

Wavenumber(cm ⁻¹)	Characteristic group
2980 broad	
1710 sharp	C=O

NMR:

Chemical shift (ppm)	Characteristic group
13	C
19	C
38	C
180	C downfield shift due to bonding to electronegative atom oxygen.

There are 4 carbons in the compound

Justification

With the mass spectrum showing a peak at 88 and an empirical formula of C₂H₄O the chemical formula of the compound is C₄H₈O₂. The peak at 29 is characteristic of a fragment formed due to the breakup of the compound in the mass spectrometer to form a C₂H₅⁺ ion. The 4 different chemical shifts indicating that the carbons are all in different environments. The peak at 180 would be due to the carbon with two oxygens bonded to it. This is consistent with the ester methyl propanoate which would have 4 different carbon environments.

