

**Mass Spec:**

m/z ratio	group
88	C <sub>2</sub> H <sub>4</sub> O is the empirical formula and has a mass of 44 so compound must have formula C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> . This is the molecular ion peak. And the base peak as it has 100% absorbance.
89	Peak due to relative isotopic abundance of <sup>13</sup> C isotope
45	COOH <sup>+</sup>
43	C <sub>3</sub> H <sub>5</sub> <sup>+</sup>
29	C <sub>2</sub> H <sub>5</sub>

**IR:**

Wavenumber(cm <sup>-1</sup> )	Characteristic group
2980 broad	Carboxylic acid
1710 sharp	C=O Aldehydes, ketones, carboxylic acids, esters

**NMR:**

Chemical shift (ppm)	Characteristic group
13	CH <sub>3</sub>
19	CH <sub>2</sub>
38	CH <sub>2</sub>
180	C downfield shift due to C bonded to highly electronegative atom or atoms

There are 4 carbons in the compound

**Justification:**

With the mass spectrum showing a peak at 88 and an empirical formula of C<sub>2</sub>H<sub>4</sub>O the chemical formula of the compound is C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>. The peak at 29 is characteristic of a fragment formed due to the breakup of the compound in the mass spectrometer to form a C<sub>2</sub>H<sub>5</sub><sup>+</sup> ion. The peak at 89 is due to isotopic abundance of the <sup>13</sup>C and will give peaks with an increased mass of 1 due to its presence in the compound. The peak at 45 is due to the COOH<sup>+</sup> ion following fragmentation as is the peak at 43 due to the C<sub>3</sub>H<sub>5</sub><sup>+</sup> ion. This indicates that compound A could be butanoic acid.

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The 4 different chemical shifts indicating that the carbons are all in different environments in the <sup>13</sup>C spectra suggest that the compound would be the straight chain butanoic acid. The peak at 180 would be due to the carbon with two oxygen atoms bonded to it. The peak at 13 is likely to be the C of the CH<sub>3</sub> group as this would be expected furthest up field and peaks at 19 and 38 due to the CH<sub>2</sub> groups between the CH<sub>3</sub> and the COOH group in the straight chain compound,

Analysis of the IR spectra shows a broad peak at  $2980\text{ cm}^{-1}$  confirming the presence of the O-H group on the butanoic acid. The acid is further confirmed by the peak at  $1750\text{ cm}^{-1}$  which is characteristic of the C=O.

The structure of A is shown below. A is butanoic acid.

