

## SL & HL Answers to Spectroscopic identification of organic compounds: Question 6

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	$48.63/12.01 = 4.05$	3
Hydrogen	$8.18 / 1.01 = 8.10$	6
Oxygen	$43.19 / 16.00 = 2.70$	2

The empirical formula of **Compound F** is  $C_3H_6O_2$

(b) The  $M^+$  peak at  $m/z = 74$  leads to the conclusion that the molar mass of **Compound F** is the same as the empirical mass so the molecular formula is  $C_3H_6O_2$ . The fragment at  $m/z 57$  is due to  $C_3H_5O^+$  due to the loss of  $-OH$  and the fragment at 45 is due to  $COOH^+$  following the loss of  $-C_2H_5$ .

(c) The very broad absorption at approximately  $3000\text{ cm}^{-1}$  shows the presence of  $-OH$  and the shoulder at about  $2950\text{ cm}^{-1}$  is due to  $C-H$ . The absorption at  $1715\text{ cm}^{-1}$  shows the presence of a carbonyl group,  $C=O$ . This supports the mass spectral data that a carboxylic acid is present in **Compound F**.

(d) The  $^1H$  NMR spectrum shows that the hydrogen atoms are in three different chemical environments. These equate to one  $-CH_3$  group (integration trace 3) one  $-CH_2-$  group (integration trace 2) and a further single hydrogen atom very far upfield at 11.5 ppm which equates to the carboxylic acid hydrogen atom. .

All this information taken together confirms that **Compound F** is **propanoic acid,  $CH_3CH_2COOH$** .

