

## SL & HL Answers to Spectroscopic identification of organic compounds: Question 5

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	$54.52/12.01 = 4.54$	2
Hydrogen	$9.17 / 1.01 = 9.08$	4
Oxygen	$36.31 / 16.00 = 2.27$	1

the empirical formula is  $C_2H_4O$

- (b) The  $M^+$  peak at  $m/z = 88$  leads to the conclusion that the molar mass of **Compound E** is twice the empirical mass and the molecular formula is  $C_4H_8O_2$ . The fragment at  $m/z 43$  is due to the loss of  $-OC_2H_5$  leaving  $CH_3CO^+$ . The fragment at 29 is due to  $C_2H_5^+$ .
- (c) The absorption at  $2984\text{ cm}^{-1}$  is due to C–H. The absorption at  $1741\text{ cm}^{-1}$  shows the presence of a carbonyl group, C=O and the absorption at  $1243\text{ cm}^{-1}$  the presence of a carbon to oxygen single bond, C–O.
- (d) The  $^1H$  NMR spectrum shows that the hydrogen atoms are in three different chemical environments. These equate to two  $-CH_3$  groups and a  $-CH_2-$  group. From the  $COC_2H_5$  fragment in the mass spectrometer it would seem that the  $-CH_2$  group is attached directly to the oxygen atom by a single bond. This is backed up by the fact that the signal due to the two hydrogen atoms is shifted upfield (4.2 ppm) away from the two  $-CH_3$  groups due to the presence of the nearby electronegative oxygen atom.

All this information taken together confirms that **Compound E** is ethyl ethanoate,  $CH_3COOCH_2CH_3$

