SL & HL Answers to Spectroscopic identification of organic compounds: Question 8

(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 of **Compound H** is C_2H_4O

(b) The M^+ peak at *m/z*= 88 leads to the conclusion that the molar mass of **Compound H** is twice the empirical mass and the molecular formula is $C_4H_8O_2$. The fragment at *m/z* = 73 is due to the loss of a methyl group $(M - CH_3)^+$ leaving $C_3H_5O_2^+$. The fragment at *m/z* = 59 is due to the loss of an ethyl group $(M - C_2H_5)^+$ leaving $C_2H_3O_2^+$ and the fragment at *m/z* = 45 is due to the loss of an propyl group $(M - C_3H_7)^+$ leaving CHO_2^+.

(c) The sharp absorption at around 3000 cm^{-1} is due to C–H. The absorption at about 1740 cm^{-1} shows the presence of a carbonyl group, C=O and the absorption at about 1190 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 four different chemical environments. These equate to one $–CH_3$ group, two $–CH_2-$ groups and one hydrogen atom bonded singly to a carbon atom to which no other alkyl groups are bonded. From the CHO_2^+ fragment in the mass spectrometer it would seem that a propyl 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 of the $–CH_2-$ group bonded to the oxygen atom is shifted upfield (4.2 ppm) away from the next $–CH_2-$ protons at 1.5 ppm followed by the methyl group at 0.9 ppm. The remaining single hydrogen atom is bonded directly to carbon atom of the carboxyl group.

All this information taken together confirms that **Compound H** is propyl methanoate, **$HCOOCH_2CH_2CH_3$**