HL Answers to Spectroscopic identification of organic compounds: Question 19

(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 S** is C_2H_4O

(b) The M^+ peak at m/z = 88 leads to the conclusion that the molar mass of **Compound S** is twice the empirical mass and the molecular formula is $C_4H_8O_2$. The fragment at m/z = 59 is due to the loss of $-C_2H_5$ leaving $CH_3CO_2^+$. The fragment at m/z = 57 is due to loss of $-OCH_3$ leaving $C_3H_5O^+$.

(c) The absorption at about 3000 cm^{-1} is due to C–H. The absorption at 1770 cm^{-1} shows the presence of a carbonyl group, C=O and the absorption at about 1200 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 loss of the $-OCH_3$ fragment in the mass spectrometer it would seem that one of the $-CH_3$ groups is attached directly to the oxygen atom by a single bond which accounts for the singlet at 3.7 ppm. The quartet and triplet at 2.3 ppm and 1.1 ppm respectively give the characteristic splitting shown by an ethyl group attached to a carbonyl group.

All this information taken together confirms that **Compound S** is **methyl propananoate, CH₃CH₂COOCH₃**.