SL & HL Answers to Spectroscopic identification of organic compounds: Question 9

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	66.61/12.01 = 5.55	4
Hydrogen	11.20 / 1.01 = 11.1	8
Oxygen	22.19 / 16.00 = 1.39	1

The empirical formula of **Compound I** is C_4H_8O

(b) The M^+ peak at m/z = 72 is evidence that the molar mass of **Compound I** is 72 g mol^{-1} and hence its molecular formula is the same as its empirical formula, C_4H_8O. The fragment at m/z = 57 is due to loss of $-CH_3$ leaving $C_3H_5O^+$ and the fragment at m/z = 43 is due to loss of $-C_2H_5$ leaving $C_2H_3O^+$. The fragment at m/z = 29 is due to $C_2H_5^+$ (it could also be due to CHO^+).

(c) The peaks at approximately 3000 cm^{-1} are due to C–H. The absorption at 1750 cm^{-1} is due to the presence of a carbonyl group, C=O.

(d) The ^1H NMR spectrum shows that the hydrogen atoms are in four different chemical environments. The fact that there is a single hydrogen atom bonded to a carbon atom containing no other hydrogen atoms bonded to it identifies the compound as an aldehyde. It suggests it is an aldehyde with two $-CH_2$ groups (the one nearest to the CO group having a shift of 2.4 ppm) and one $-CH_3$ group with a shift of 0.9 ppm..

All this information taken together confirms that **Compound I** is **butanal, $CH_3CH_2COCH_3$**.