SL & HL Answers to Spectroscopic identification of organic compounds: Question 3

(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 C** is C_4H_8O

(b) The M^+ peak at m/z = 72 is evidence that the molar mass of **Compound C** 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 1705 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 three different chemical environments. None of them indicate a single hydrogen atom on its own so the compound cannot be an aldehyde. It suggests it is a ketone with two $–CH_3$ groups and one $-CH_2$ group. This is confirmed by the upfield chemical shifts of the signals due to the two groups $–COCH_3$ and $–CH_2CO$ (2.0 ppm and 2.3 ppm respectively)) relative to the 0.9 ppm shift of the methyl group next to the $–CH_2$ group.

All this information taken together confirms that **Compound C** is butanone, **$CH_3CH_2COCH_3$**