HL Answers to Spectroscopic identification of organic compounds: Question 15

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	71.93/12.01 = 5.99	6
Hydrogen	12.10 / 1.01 = 11.98	12
Oxygen	15.97 / 16.00 = 1.00	1

The empirical formula of **Compound O** is $C_6H_{12}O$

(b) The M^+ peak at m/z = 100 is evidence that the molar mass of **Compound O** is 100 g mol^{-1} and hence its molecular formula is the same its empirical formula, i.e. $C_6H_{12}O$. The fragment at m/z = 71 is due to loss of either –CHO or $–CH_2CH_3$ i.e. $(M – CHO)^+$ or $(M – C_2H_5)^+$ and the fragment at m/z = 29 is due to CHO^+ or $C_2H_5^+$. (Although not on the IB syllabus the fragment at m/z = 72 is due to H^+ recombining after loss of an ethyl group to form $C_2H_5CHCHOH^+$ and the fragment at m/z = 43 is due to $–CHCHOH^+$ after the loss of the second ethyl group).

(c) The absorptions at just below 3000 cm^{-1} are due to C–H and the sharp absorption at 1730 cm^{-1} is due to the presence of a C=O. double bond.

(d) The ^1H NMR spectrum shows that the hydrogen atoms are in four different chemical environments. The position of the single proton split into a doublet with a shift of 9.6 ppm is indicative of an aldehyde –CHO adjacent to a C atom containing one H atom. This means that **Compound O** is an isomer of hexanal. The triplet at 0.9 ppm (due to $-CH_3$) and the complex signal at 1.6 ppm (due to $-CH_2-$) indicate two ethyl groups. These are both bonded to a carbon atom bonded to one hydrogen atom (hence the complex splitting pattern) and the aldehyde functional group which gives the complex pattern for a single proton at 2.1 ppm.

All this information taken together confirms that **Compound O** is **2-ethylbutanal, $(C_2H_5)_2CHCHO$**.