SL & HL Answers to Spectroscopic identification of organic compounds: Question 7

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	83.60/12.01 = 6.96	3
Hydrogen	16.40 / 1.01 = 16.24	7

The empirical formula of **Compound G** is C_3H_7

(b) The M^+ peak at m/z = 86 gives a mass equal to twice that of the empirical mass so the molecular formula is C_6H_{14} which means **Compound G** is an isomer of hexane. The fragment with the *m/z* value of 71 is due to the loss of one methyl group $(M - CH_3)^+$, i.e. $C_5H_{11}^+$. The fragment at *m/z* = 57 is due to the loss of one ethyl group $(M - C_2H_5)^+$, i.e. $C_4H_9^+$.and the fragment at *m/z* = 43 is due to the loss of one propyl group $((M - C_3H_7)^+$, i.e. $C_3H_7^+$.

(c) The strong sharp absorption at just below 3000 cm^{-1} shows the presence of the C–H bonds in the alkane.

(d) The ^1H NMR spectrum shows that the fourteen hydrogen atoms are in five different chemical environments. From the ratios of the signals six of the hydrogen atoms are in identical environments – this suggests that it contains two methyl groups in identical chemical environments. One carbon atom is bonded to just one hydrogen atom so the compound is therefore either 2-methylpentane or 3-methylpentane as both compounds have one hydrogen atom in a separate chemical environment. 3-methylpentane is more symmetrical as it contains two CH_3CH_2– groups in the same chemical environment and would only give four signals in the ratio of 1:3:4:6, whereas 2-methylpentane will give five signals in the ratio 1:2:2:3:6.

All this information taken together confirms that **Compound G** is **2-methylpentane**, **$(CH_3)_2CHCH_2CH_2CH_3$**.