HL Answers to Spectroscopic identification of organic compounds: Question 18

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	37.82/12.01 = 3.15	2
Hydrogen	6.36 / 1.01 = 6.30	4
Chlorine	55.82 / 35.45 = 1.57	1

The empirical formula of **Compound R** is C_2H_4Cl

(b) The M^+ peak at m/z = 126 is evidence that the molar mass of **Compound R** is 126 g mol^{-1} and hence its molecular formula is twice its empirical formula, i.e. $C_4H_8Cl_2$. 126 g mol^{-1} is the molar mass when the isotopes of the two chlorine atoms are both ^{35}Cl. The peak at m/z = 128, the $(M+2)^+$ peak, is when one of the Cl atoms is ^{35}Cl and the other ^{37}Cl. The peak at m/z = 140, the $(M+4)^+$ peak, is when both of the chlorine atoms are ^{37}Cl. The fragment at m/z = 63 is due to the molecule being split in half to give $C_2H_4{}^{35}Cl^+$. The smaller peak at at m/z = 65 is due to $C_2H_4{}^{37}Cl^+$. The fragment at m/z = 62 is due to loss of a further proton to give $C_2H_3{}^{35}Cl^+$ with a smaller peak for the analogous fragment containing the other isotope of chlorine, $C_2H_3{}^{37}Cl^+$ at m/z = 64. From its molecular formula **Compound R** and its fragmentation pattern the molecule looks to be a symmetrical dichloroalkane.

(c) The absorptions at approximately 3000 cm^{-1} are due to C–H and the absorption at 650 cm^{-1} is likely to be due to the presence of a C−Cl single bond.

(d) The ^1H NMR spectrum shows that the eight hydrogen atoms are in two different chemical environments in the ratio 3:1. The doublet centred at at 1.6 ppm suggests two separate methyl groups each attached to a carbon atom containing one H atom. Similarly the complex doublet centred at 4.1 ppm suggests two C-H entities each attached to a $–CH_3$ group and to a -C−H entity.

All this information taken together confirms that **Compound R** is **2**, **3-dichlorolbutane, $CH_3CHClCHClCH_3$**.