SL & HL Answers to Spectroscopic identification of organic compounds: Question 1

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	24.3/12.01 = 2.02	1
Hydrogen	4.1 / 1.01 = 4.05	2
Chlorine	71.6 / 35.45 = 2.02	1

the empirical formula is CH_2Cl

(b) From the mass spectrum the molar molecular mass is either 98, 100 or 102 g mol^{-1}. This means that it is twice the empirical mass (49.48 g mol^{-1}) and so the molecular formula is $C_2H_4Cl_2$. The three different molar masses are due to the molecule containing isotopes of chlorine. For M^+ = 98 both will be ^{35}Cl, for M^+ = 100 one will be ^{35}Cl and the other ^{37}Cl and for M^+ = 102 both will be ^{37}Cl. The peak at m/z = 63 will be due to loss of ^{35}Cl (98-35 = 63) and the peak at m/z = 83 will be due to loss of a $–CH_3$ fragment leaving $CHCl_2^+$. (Peaks due to isotopes are not on the syllabus but this does not seem too difficult for students to comprehend).

(c) The peak at 2989 cm^{-1} is due to C-H. No other helpful information can be obtained. (In fact the peak at 750 cm^{-1} in the fingerprint region is probably due to C-Cl, but this is not on the syllabus).

(d) The integration trace shows that three of the hydrogen atoms are in the same environment suggesting a $–CH_3$ group and that one is in an environment on its own suggesting $–CHCl_2$. This is confirmed by the upfield chemical shift (5.8 ppm) of this signal relative to the $–CH_3$ shift (2.0 ppm).

All this information taken together confirms that **Compound A** is **1,1-dichloroethane, CH_3CHCl_2**.