SL & HL Answers to Spectroscopic identification of organic compounds: Question 2

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	15.40/12.01 = 1.28	2
Hydrogen	3.24 / 1.01 = 3.21	5
Iodine	81.36 / 126.90 = 0.641	1

the empirical formula is C_2H_5I

(b) The M^+ peak at 156 is evidence that the molar molecular mass of **Compound B** is 156 g mol^{-1} and hence its molecular formula is the same as its empirical formula. The fragment at $m/z = 27$ is due to I^+ and the fragment at $m/z = 29$ is due to $C_2H_5^+$. (In fact there is only one compound that can have the formula C_2H_5I so the compound must be iodoethane).

(c) The peaks at approximately 3000 cm^{-1} are due to C–H. No other helpful information can be obtained. (The peak at 1200 cm^{-1} in the fingerprint region is probably due to C–I, 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 the other two are in a separate environment which suggests –CH_2I. This is confirmed by the upfield chemical shift (3.1 ppm) of this signal (due to the more electronegative iodine atom) relative to the –CH_3 shift (1.8 ppm).

All this information taken together confirms that **Compound B** is **iodoethane, CH_3CH_2I**