SL & HL Answers to Spectroscopic identification of organic compounds: Question 4

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	29.29/12.01 = 2.44	3
Hydrogen	5.75 / 1.01 = 5.69	7
Bromine	64.96 / 79.91 = 0.813	1

the empirical formula is C_3H_7Br

(b) The M^+ peaks at 122 and 124 leads to the conclusion that the molar mass of **compound D** is the same as the empirical mass and the molecular formula is C_3H_7Br. There are two peaks due to the two isotopes of bromine ^{79}Br and ^{81}Br (which are present in roughly equal amounts to give an actual molar mass for **Compound D** of 123 .01 g mol^{-1}). The fragment at m/e 43 is due to loss of bromine leaving $C_3H_7^+$.

(c) The absorption at 2987 cm^{-1} is due to C–H. Absorptions due to C–Br are not on the syllabus and no other information can be obtained from the infrared spectrum without computer analysis of the fingerprint region.

(d) The ^1H NMR spectrum shows that the hydrogen atoms are in two different chemical environments. One of them indicates a single hydrogen atom which suggests –CHBr- and the six other hydrogen atoms suggest that there are two $–CH_3$ groups attached to this central carbon atom. This is confirmed by the relative upfield chemical shift of the signal due to the single hydrogen atom bonded to the carbon atom containing the bromine atom at 4.3 ppm relative to the 1.7 ppm shift of the hydrogen atoms in the two methyl groups.

All this information taken together confirms that **Compound D** is 2-bromopropane **$CH_3CHBrCH_3$**.