HL Answers to Spectroscopic identification of organic compounds: Question 20

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	85.60/12.01 = 7.13	1
Hydrogen	14.40 / 1.01 = 14.26	2

The empirical formula of **Compound T** is CH_2.

(b) The M^+ peak at *m/z* = 70 gives a mass equal to five times that of the empirical mass so the molecular formula is C_5H_{10}. The peak with the *m/z* value of 55 suggests loss of a methyl group to give the $C_4H_7^+$ fragment. Loss of an ethyl group $(M - C_2H_5)^+$, i.e. $C_3H_5^+$ is likely to have produced the peak at m/z = 41.

(c) The strong sharp absorptions at just below 3000 cm^{-1} show the presence of the C–H bonds. The sharp absorption at 1651 cm^{-1} suggests a C=C double bond so **Compound T** is an alkene.

(d) The ^1H NMR spectrum shows that the ten hydrogen atoms are in four different chemical environments in the ratio 2:2:3:3. The singlet at 4.6 ppm has the chemical shift due to –CH=C**H**$_2$ which suggest the double bond is on the first carbon atom which is bonded to two hydrogen atoms. The singlet at 1.6 ppm suggests a methyl group attached to a carbon atom containing no hydrogen atoms bonded to it. The quartet and triplet at 2.0 ppm and 1.0 ppm respectively are indicative of an ethyl group attached to the other carbon atom of the double bond.

All this information taken together confirms that **Compound T** is **2-methylbut-1-ene**, **$H_2C=C(CH_3)C_2H_5$.**