HL Answers to Spectroscopic identification of organic compounds: Question 11

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	28.76/12.01 = 2.39	4
Hydrogen	4.23 / 1.01 = 4.19	7
Oxygen	19.16 / 16.00 = 1.20	2
Bromine	47.85 / 79.91 = 0.599	1

the empirical formula of **Compound K** is $C_4H_7O_2Br$.

(b) The two M^+ peaks at m/z = 166 and 168 are due to the two isotopes of bromine, ^{79}Br and ^{81}Br which are present in roughly equal amounts. The average value for the molar mass of 167 g mol^{-1} is the same as the value for the empirical formula so the molecular formula of **Compound K** is $C_4H_7O_2Br$. The fragment at m/z = 87 is due to what remains after a bromine atom has been removed, i.e. $C_4H_7O_2^+$.

(c) The very broad absorption at approximately 3000 cm^{-1} shows the presence of –OH. Together with the C=O absorption at 1707 cm^{-1} this suggests the presence of a carboxylic acid. The sharp peaks (shoulders) at around 3000 cm^{-1} are due to C-H.

(d) The ^1H NMR spectrum shows that the seven hydrogen atoms are in two different chemical environments. The singlet very high upfield at 12.0 ppm is due to the carboxylic acid proton (this is confirmed by the fact that it exchanges with D_2O. The remaining six hydrogen atoms are all in the same chemical environment and the signal is a singlet suggesting two methyl groups bonded to a carbon atom which contains no hydrogen atom bonded directly to it.

All this information taken together confirms that **Compound K** is
2-bromo-2-methylpropanoic acid, **$(CH_3)_2CBrCOOH$**.