HL Answers to Spectroscopic identification of organic compounds: Question 13

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	68.11/12.01 = 5.67	5
Hydrogen	13.74 / 1.01 = 13.60	12
Oxygen	18.15 / 16.00 = 1.13	1

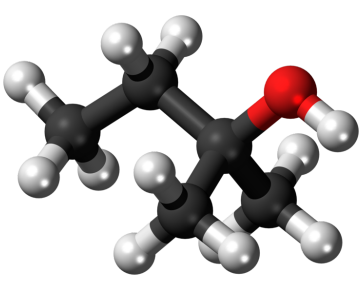
The empirical formula of **Compound M** is $C_5H_{12}O$

(b) Presumably the M^+ ion is not very stable nevertheless its m/z value of 88 means that the empirical and molecular mass are the same so the molecular formula of **Compound M** is $C_5H_{12}O$. The peak at m/z = 73 shows loss of a $–CH_3$ group to give the fragment $C_4H_9O^+$. $–CH_2$ can then also be lost to leave the fragment $C_3H_7O^+$ that is responsible for the peak at m/z = 59.

(c) From its molecular formula **Compound M** could either be an alcohol or an ether. The very broad absorption centred at 3376 cm^{-1} shows the presence of an –OH group so **Compound M** is an alcohol. The only other peaks that are easy to attribute are the absorptions centred at about 3000 cm^{-1} which are due to C-H.

(d) The integration trace shows that the twelve hydrogen atoms are in four different chemical environments in the ratio of 1:2:6:3. The singlet at 2.8 ppm accounts for the hydrogen atom of the alcohol group. The large singlet due to six protons centred at 1.2 ppm suggests two $–CH_3$ groups attached to a carbon atom that has no hydrogen atoms attached to it. The quartet at 1.5 ppm and the triplet at 0.9 ppm represent the $–CH_2$ and the $–CH_3$ constituents of an ethyl group respectively. Because the quartet due to the $–CH_2$ group is not split further this means that the ethyl group is also attached to a carbon atom to which no other hydrogen atoms are attached.

All this information taken together confirms that **Compound M** is **2-methylbutan-2-ol**, **$CH_3CH_2C(CH_3)_2OH$**.



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