HL Answers to Spectroscopic identification of organic compounds: Question 17

(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

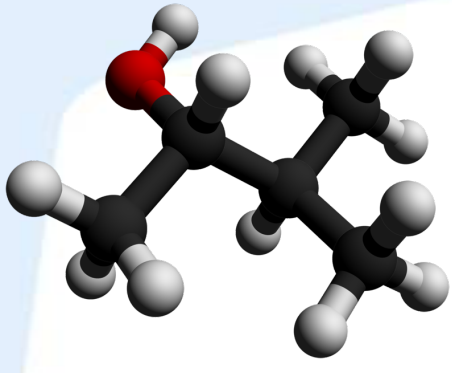
The empirical formula of **Compound Q** is $C_5H_{12}O$

(b) The M^+ peak at m/z = 88 is evidence that the molar mass of **Compound Q** is 88 g mol^{-1} and hence its molecular formula is the same as its empirical formula, $C_5H_{12}O$. The fragment at m/z = 73 is due to loss of an methyl group, $-CH_3$ leaving $C_4H_9O^+$. The fragment at m/z = 45 is due loss of $-C_2H_5O$ leaving $C_3H_7^+$ with the peak a at m/z = 43 due to $C_2H_5O^+$.

(c) From its molecular formula **Compound Q** could either be an alcohol or an ether. The broad absorption at about 3300 cm^{-1} is indicative of the presence of an –OH bond and hence **Compound Q** is an alcohol. The peaks at approximately 3000 cm^{-1} are due to C–H. The absorption at 1050 cm^{-1} is likely to be due to the presence of a C−O single bond.

(d) The ^1H NMR spectrum shows that the twelve hydrogen atoms are in five different chemical environments in the ratio 6:3:1:1:1. The doublet at 0.9 ppm suggests two methyl groups attached to a carbon atom containing one H atom. Similarly the doublet at 1.1 ppm suggests one methyl group attached to a carbon atom containing one H atom. The two protons with complex splitting patterns with integration traces of one indicate two separate C−H entities bonded to adjacent carbon atoms that contain more than three protons. The one at 3.6 ppm is due to the C−H proton adjacent to the carbon atom containing the −OH group. The remaining singlet at 1.8 ppm is due to the hydrogen atom of the –OH group as this will not be split.

All this information taken together confirms that **compound Q** is **3-methylbutan-2-ol, $CH_3CH(OH)CH(CH_3)_2$.**



© Dr Geoffrey Neuss, InThinking
http://www.thinkib.net/chemistry