HL Answers to Spectroscopic identification of organic compounds: Question 14

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	54.52/12.01 = 4.54	2
Hydrogen	9.17 / 1.01 = 9.08	4
Oxygen	36.31 / 16.00 = 2.27	1

The empirical formula of **compound N** is C_2H_4O

(b) The M^+ peak at m/z = 88 leads to the conclusion that the molar mass of **compound N** is twice the empirical mass and the molecular formula is $C_4H_8O_2$. The fragment at m/z = 73 suggests loss of a methyl group to leave $C_3H_5O_2^+$, the fragment at m/z = 45 could either be due to $COOH^+$ or due to CH_3CHOH^+ and the fragment at m/z = 43 is probably due to either $C_3H_7^+$ or $COCH_3^+$.

(c) The very broad absorption centred at 3428 cm^{-1} is due to the –OH of an alcohol and the sharp peak just below 3000 cm^{-1} is due to C–H absorption. The absorption at 1714 cm^{-1} shows the presence of a carbonyl group, C=O.

(d) The ^1H NMR spectrum shows that the hydrogen atoms are in four different chemical environments. The single very broad absorption at approximately 3.5 ppm that exchanges with heavy water may be due to the hydrogen atom of the alcohol group. The doublet at 1.4 ppm corresponds to a methyl group split by one adjacent hydrogen atom on the next carbon atom. This adjacent hydrogen atom will be split by the methyl group into a quartet that accounts for the signal at 4.3 ppm. The remaining signal at 2.2 ppm is a singlet and is due to a methyl group with no hydrogen atoms bonded to the carbon atom next to it.

All this information taken together confirms that **Compound N** is **3-hydroxybutan-2-one, $CH_3CH(OH)COCH_3$**.