

HL Answers to Spectroscopic identification of organic compounds: Question 12

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	$80.56/12.01 = 6.71$	9
Hydrogen	$7.52 / 1.01 = 7.45$	10
Oxygen	$11.92 / 16.00 = 0.745$	1

The empirical formula of **Compound L** is $C_9H_{10}O$

(b) The M^+ peak at $m/z = 134$ leads to the conclusion that the molar mass of **Compound L** is the same as the empirical mass and so the molecular formula is $C_9H_{10}O$. The fragment at $m/z = 105$ suggests loss of an ethyl group to leave $C_7H_5O^+$, the fragment at $m/z = 77$ is likely to be due to $C_6H_5^+$ which strongly suggests a phenyl group is present in the molecule.

(c) The absorption centred just below 3000 cm^{-1} is due to C–H absorption. The absorption at 1690 cm^{-1} shows the presence of a carbonyl group, C=O.

(d) The ^1H NMR spectrum essentially shows that the hydrogen atoms are in three different chemical environments as the trace of two and three at 7.5 ppm and 8 ppm respectively represent the five phenyl hydrogen atoms. The quartet at 2.9 ppm and the triplet at 1.2 ppm are characteristic of the $-CH_2-$ and $-CH_3$ respectively of an ethyl group.

All this information taken together confirms that **Compound L** is **propiophenone** (ethyl phenyl ketone), $C_6H_5COC_2H_5$.

