SL & HL Answers to Spectroscopic identification of organic compounds: Question 10

(a) From the elemental analysis

Element	Amount / mol	Simplest ratio
Carbon	70.56/12.01 = 5.88	4
Hydrogen	5.93 / 1.01 = 5.87	4
Oxygen	23.51 / 16.00 = 1.47	1

The empirical formula of **Compound J** is C_4H_4O

(b) The M^+ peak at m/z = 136 is evidence that the molar mass of **Compound J** is 136 g mol^{-1} and hence its molecular formula is twice its empirical formula, i.e. $C_8H_8O_2$. The fragment at m/z = 91 is due to loss of $–CO_2H$ leaving $C_7H_7^+$ and the fragment at m/z = 77 is due to loss of $–CH_2CO_2H$ leaving $C_6H_5^+$.

(c) The absorptions at approximately 3000 cm^{-1} are due to C–H and the sharp absorption at just below 1800 cm^{-1} is due to the presence of a C=O. bond. The absorption at approximately 1100 cm^{-1} is due to the C–O single bond. The broad absorption just below 3000 cm^{-1} in the liquid phase signifies a carboxylic acid with hydrogen bonding. (This broad absorption occurs in the liquid state as it is due to the vibrational stretching of the intermolecular hydrogen bonds that occurs between molecules, as carboxylic acids dimerize in the liquid state. In the gaseous state this absorption is absent as the molecules will have sufficient energy and be too far apart for this hydrogen bonding to occur.)

(d) The ^1H NMR spectrum shows that the hydrogen atoms are in three different chemical environments. The position of the single proton with a shift of 10.8 ppm is indicative of a carboxylic acid, –COOH. The five protons with a shift of 7.4 ppm suggest a phenyl group, $C_6H_5–$ and the remaining two protons with a chemical shift of 3.7 ppm suggest a $–CH_2–$ group bonded between the phenyl group and the carboxylic acid group.

All this information taken together confirms that **Compound J** is **phenylethanoic acid, $C_6H_5CH_2COOH$**.