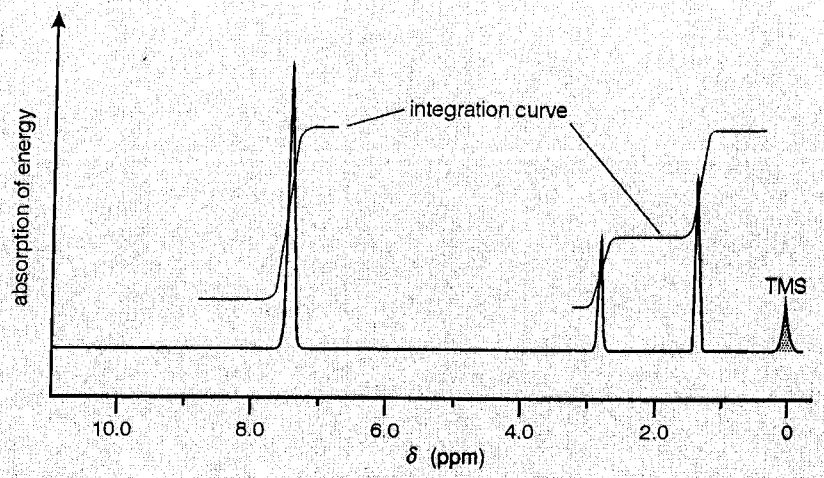
Pages 89–90

Refer to the spectra on pages 89–90 of *Unit 3: Organic Chemistry*.

Question 1

From the following low-resolution NMR spectra and other information given, suggest a possible structure for each substance.
Figure 119 shows the ^1H NMR spectrum of a hydrocarbon.

Figure 119



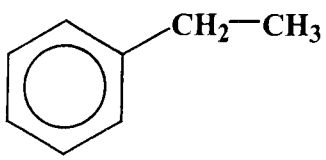
Answer

There are three signals and so there must be three different environments for the hydrogen atoms. The integral will give the ratio of the atoms causing the signals.

Chemical shift	Integral	Ratio
7.4 δ	23 mm	5
2.8 δ	9 mm	2
1.4 δ	14 mm	3

Using the correlation tables on page 15 of the Data Booklet, the signal at 7.4 δ (caused by 5 hydrogen atoms) corresponds to aromatic hydrogen atoms. This is likely to be caused by C_6H_5–, a mono-substituted benzene ring.

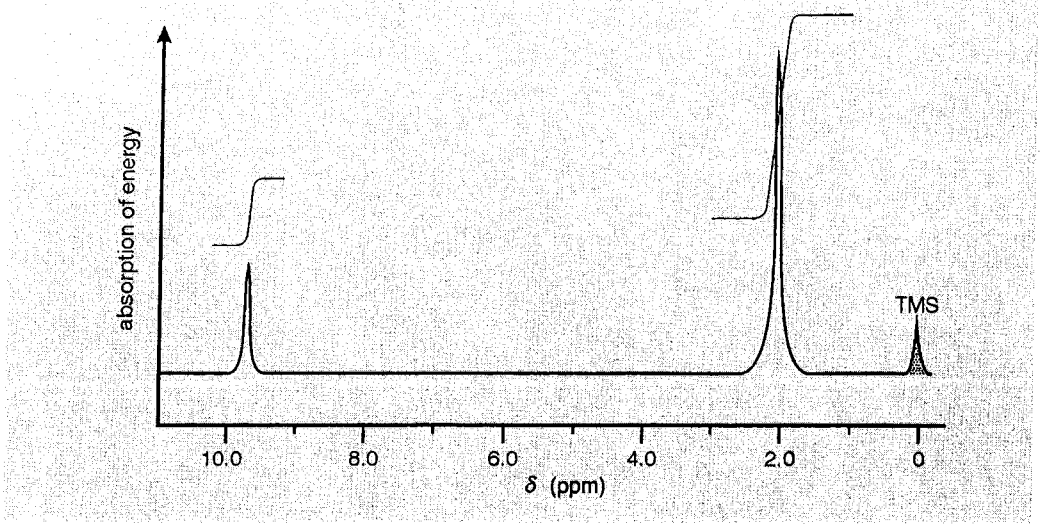
The signal at 1.4 δ is likely to be caused by a methyl group, CH_3–, while that at 2.8 δ is likely to be from a $-CH_2-$ group.
Putting this all together gives ethylbenzene.



Question 2

Figure 120 is the spectrum produced by a compound of molecular formula C_2H_4O. Suggest a possible structure for the compound.

Figure 120

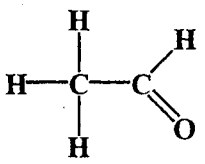


Answer

There are two signals. So there are two different environments for the hydrogen atoms.

Chemical shift	Integral	Ratio	Type of hydrogen
2.1 δ	25.5 mm	3	methyl group
9.7 δ	8.5 mm	1	aldehyde

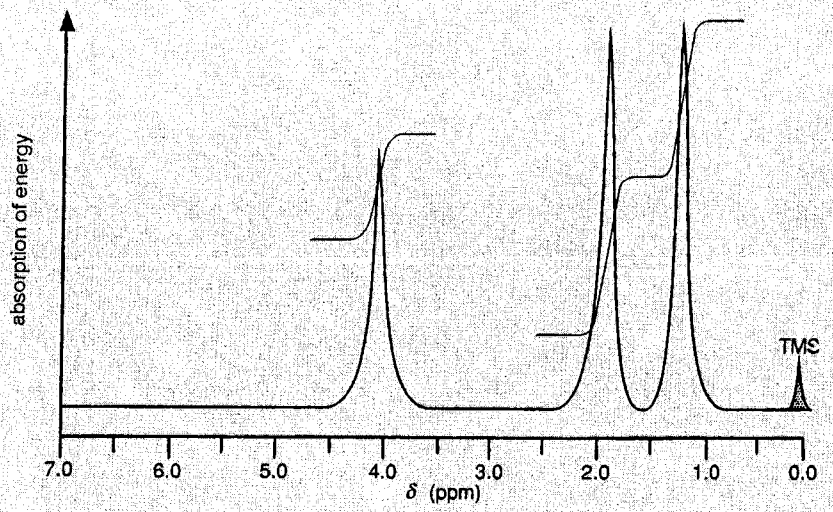
Putting this together gives ethanal.



Question 3

Analysis of a sweet-smelling neutral compound of carbon, hydrogen and oxygen produced the following results: %C = 54.5; %H = 9.1. From its mass spectrum, the molecular ion had a mass/charge ratio of 88. Its infra-red spectrum showed a prominent peak at 1735 cm^{-1}. Figure 121 shows the NMR spectrum of the compound. Suggest a possible structure for the compound.

Figure 121



Answer

First calculate the empirical formula.

	C	H	O
Mass in 100 g	54.5 g	9.1 g	36.4 g
Relative atomic mass	12	1	16
Moles	4.425	9.1	2.275
Ratio	4.425/2.275	9.1/2.275	2.275/2.275
	= 2	= 4	= 1

The empirical formula is C_2H_4O. The formula mass of C_2H_4O is 44.

The molecular ion shows a molecular mass of 88. So the molecular formula is twice the empirical formula, i.e. $C_4H_8O_2$.

The infra-red spectrum contains a peak at 1735 cm^{-1} which suggests the presence of a carbonyl group, C=O.

The NMR spectrum shows three signals and so three different types of hydrogen atom.

Chemical shift	Integral	Ratio
4.1 δ	13 mm	2
1.9 δ	20 mm	3
1.2 δ	20 mm	3

From the correlation tables, the signals at 1.2 and 1.9 δ are likely to be produced by methyl groups. The signal at 4.1 δ (caused by two hydrogens) is likely to be due to a $-CH_2-$ group. This signal has quite a high δ value for a $-CH_2-$ group and so is likely to be adjacent to an oxygen atom (see correlation tables in the Data Booklet).

Summarising, the molecule contains the following:

$C=O \quad CH_3- \quad CH_3- \quad -CH_2O-$

This is consistent with the molecular formula of $C_4H_8O_2$. Putting the pieces together, the molecule is likely to be ethyl ethanoate.