

TOPIC 20 EXERCISE 4 – COMBINED SPECTRAL ANALYSIS

1. A compound containing 58.8% carbon, 9.8% hydrogen and 31.4% oxygen is subjected to mass spectrometry and found to a molecular ion peak at $m/z = 102$.

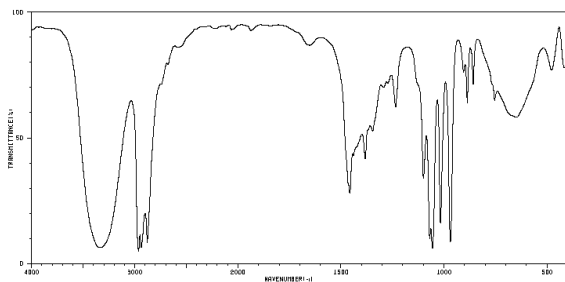
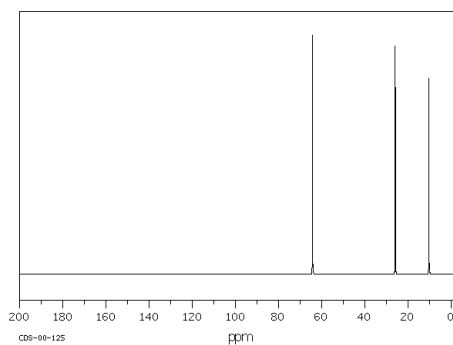
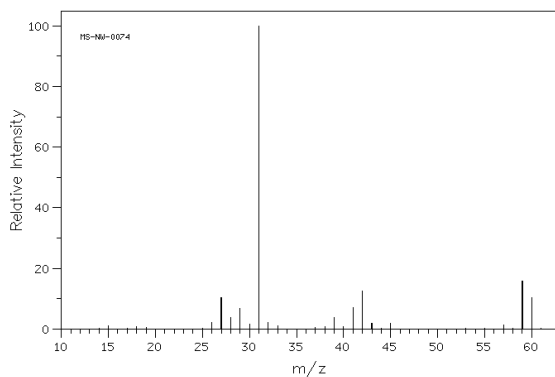
Infra-red analysis of the molecule showed a sharp peak at $m/z = 1710 \text{ cm}^{-1}$.

A proton nmr spectrum of the molecule yielded the following peaks:

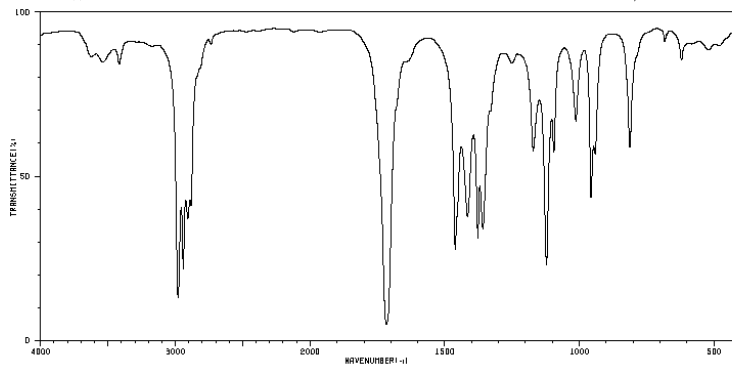
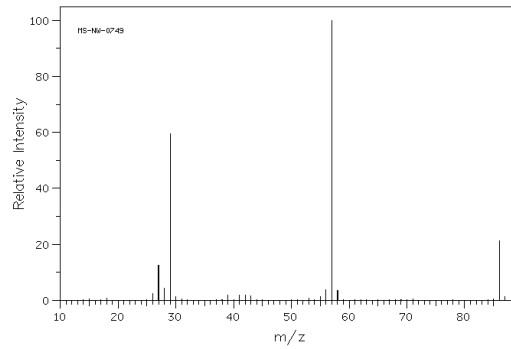
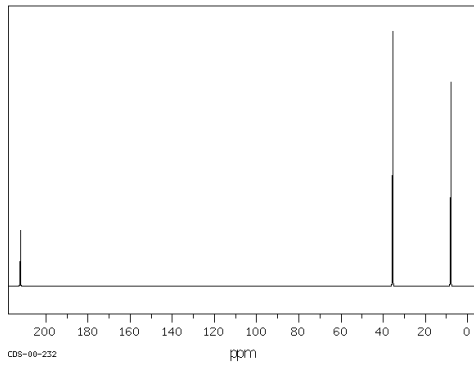
Chemical shift	Splitting	Integration factor
0.8	Triplet	3
1.1	Sextet	2
2.3	Triplet	2
3.7	Singlet	3

Deduce the structure of the molecule and account for the formation of all the peaks in the spectra.

2. Identify this molecule:



3. Identify this molecule:



SOLUTIONS

1. empirical formula = $C_5H_{10}O_2$
from mass spectrum $m_r = 102$, $e_{fm} = 102$ so $m_f = C_5H_{10}O_2$
infra-red spectrum:
peak at 1710 cm^{-1} indicates a carbonyl
proton nmr spectrum:
peak at 0.8 is CH_3 - adjacent to $-CH_2-$
peak at 1.1 is $-CH_2-$ adjacent to CH_3 - and $-CH_2-$
peak at 2.3 is $-CH_2CO-$ adjacent to $-CH_2-$
peak at 3.7 is CH_3O-
so molecule is methyl butanoate, $CH_3CH_2CH_2COOCH_3$
2. from mass spectrum $m_r = 60$
From ^{13}C nmr 60 ppm = C-O (alcohol)
 3300 cm^{-1} in IR spectrum confirms -OH alcohol
 $C_nH_{2n+2}O = 60$ so $n = 3$
No identical C environments so must be $CH_3CH_2CH_2OH$ (propan-1-ol)
3. from mass spectrum $m_r = 86$
From ^{13}C nmr 220 ppm = C=O (carbonyl)
 1700 cm^{-1} in IR spectrum confirms C=O
 $C_nH_{2n}O = 86$ so $n = 5$
Three C environments only so either $(CH_3)_3CCHO$ (dimethylpropanal) or
 $CH_3CH_2COCH_2CH_3$ (pentan-3-one)