

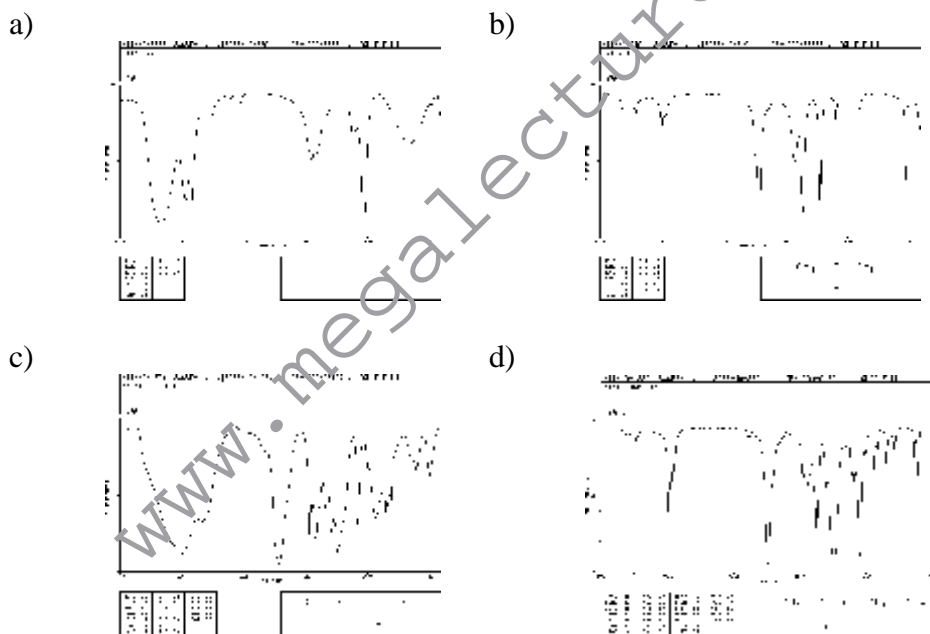


2.11 EXERCISE 1 – Analytical Techniques

1.
 - a) Low resolution mass spectrometry identified the molecular ion peak of an organic molecule as 86. Suggest three possible molecular formulae for the molecule.
 - b) High resolution mass spectrometry identified the molecular ion peak of the organic molecule as 85.998. Deduce the molecular formula of the molecule, given the following relative isotopic masses:

isotope	Relative isotopic mass
^{16}O	15.994
^{12}C	12.000
^1H	1.008

2. Identify the bonds responsible for all the peaks in the non-fingerprint region of the following infra-red spectra, and hence state the functional group present:



3. Three compounds A, B and C, all with molecular formula $\text{C}_4\text{H}_8\text{O}_2$, are found to have very different infra-red spectra. All three spectra contain a sharp peak at 1700 cm^{-1} , but the infra-red spectrum of A contains a broad peak at $2500 - 3000\text{ cm}^{-1}$, the infra-red spectrum of B contains no broad peaks, and the infra-red spectrum of C contains a broad peak at $3000 - 3300\text{ cm}^{-1}$. Suggest possible structures for A, B and C.



4. Suggest how infra-red spectroscopy could be used to determine the exact structure of a molecule containing only C-H absorptions and a C=O absorption in the region $1500 - 3500 \text{ cm}^{-1}$.