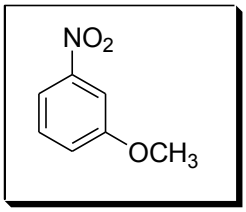
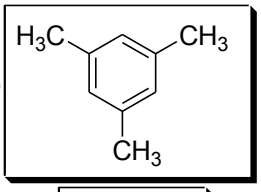
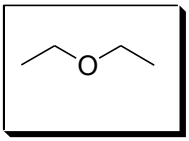
Practice Problems

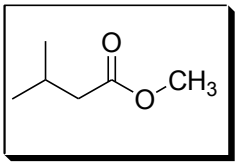
1. Please find the number of NMR signals, splitting and their relative chemical shifts for the following molecules (Any five): 5*3 = 15

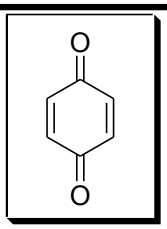
   There is one illustration given for you. No further explanation is required.

(a) 

(b) 

(c) 

(d) 

(e) 

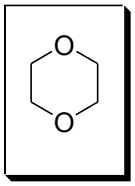
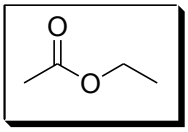
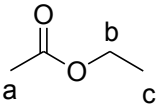
(f) 

Illustration:-

(x) 

Answer:

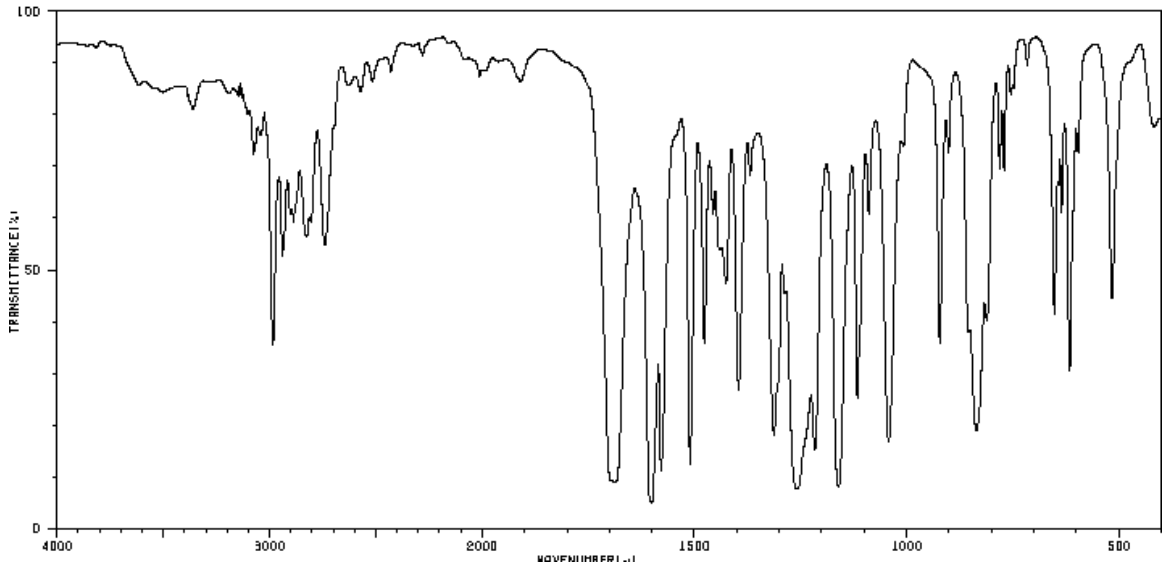
Number of signals = 3

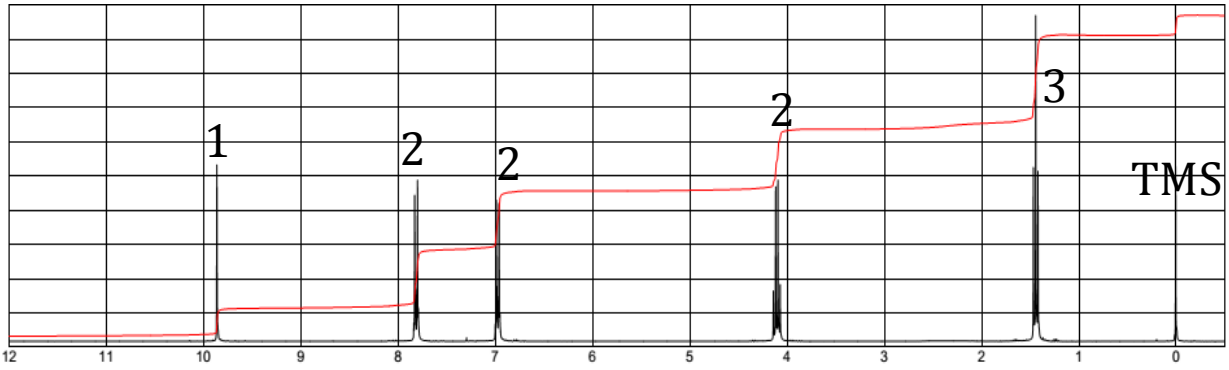
Assignment = 

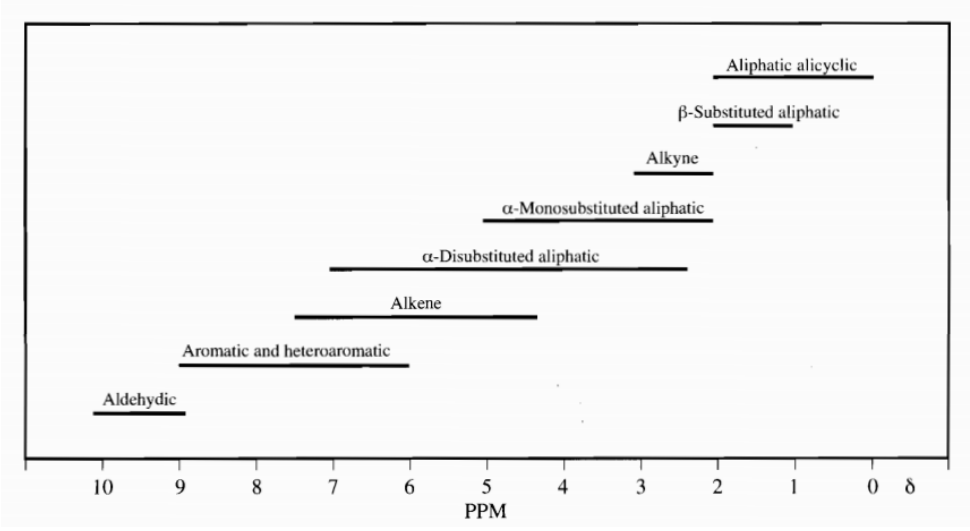
Splitting pattern = For a, singlet (s), for b, quartet (q) and for c, triplet (t)

Relative order of chemical shift = $\delta_b > \delta_a > \delta_c$

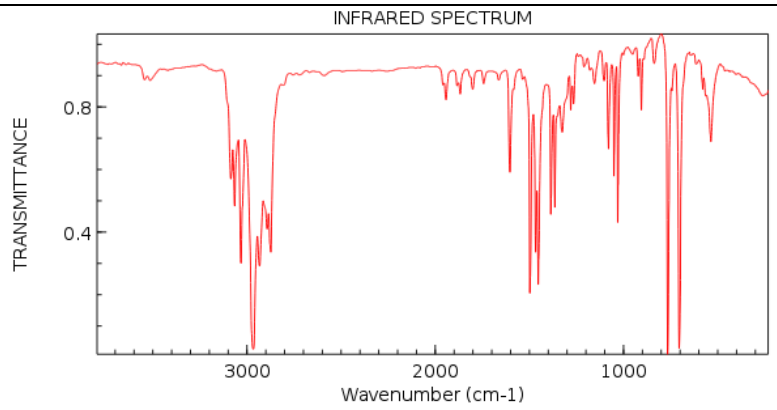
2. Assign the structure of the molecule ($C_9H_{10}O_2$) from the molecular formula, IR and NMR spectrum. 5

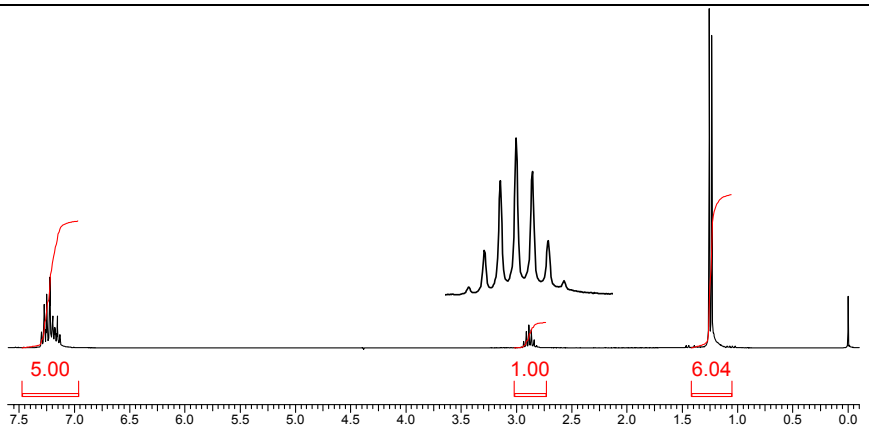






3. Predict the structure of the molecule with a molecular formula C_9H_{12} based on the available spectral data: (Assign the NMR spectral data based on the predicted structure)





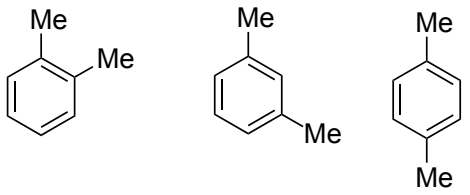
^{1}H-NMR (CDCl3, 400 MHz)

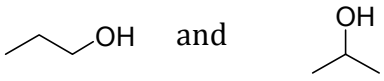
δ (ppm): 1.24 (d, *J*=6.9 Hz, 6H),

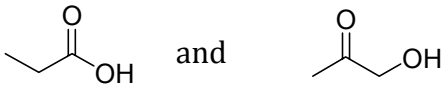
2.87 (septet, *J*=6.9 Hz, 1H),

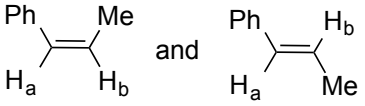
7.02 - 7.39 (m, 5H)

Q2. (a) How to distinguish the following sets of isomeric species using NMR spectroscopy?

(i) 

(iii) 

(ii) 

(iv) 

Q3. Predict the number of signals, first order splitting pattern and approximate chemical shift for the following molecules: (Consider that all the spectra are recorded at rt)

(a) Triethylamine (b) N,N-Dimethyl formamide (c) 4-Methoxy benzaldehyde