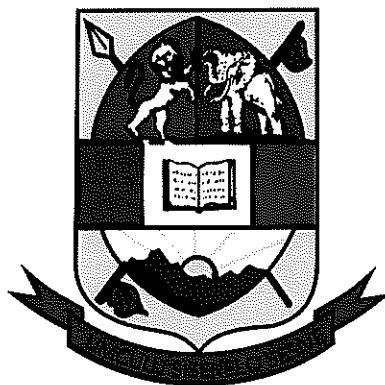


UNIVERSITY OF ESWATINI**Applied Spectroscopy – 2019/2020**

TITLE OF PAPER: Applied Spectroscopy

COURSE NUMBER: CHE 602

TIME ALLOWED: Three Hours

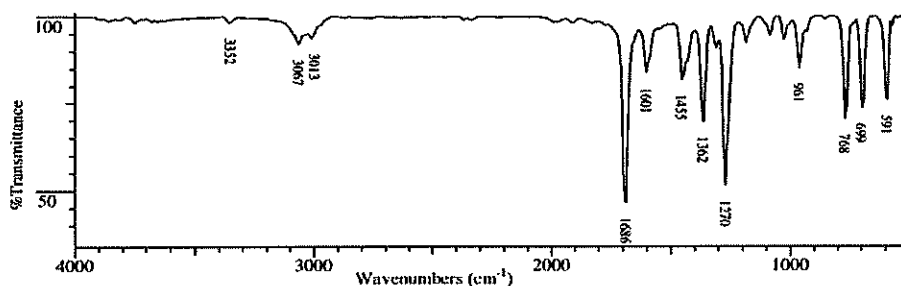
INSTRUCTIONS:

Answer any four (4) questions of the six (6) questions and every question holds 25 marks. NB: all questions are to be answered in a separate answer sheet.

Please do not open this paper until authorised to do so by the Chief Invigilator.

Question A

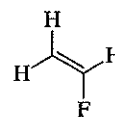
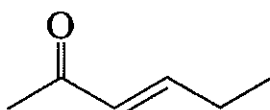
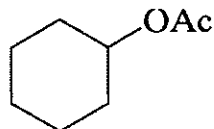
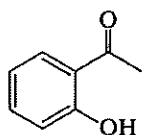
- 1) What information can one extract from the EI and CI spectra? (5)
- 2) Compare CI ionization and EI ionization in mass spectrometry? (4)
- 3) What functional groups can you establish from the IR spectrum below?
(6)



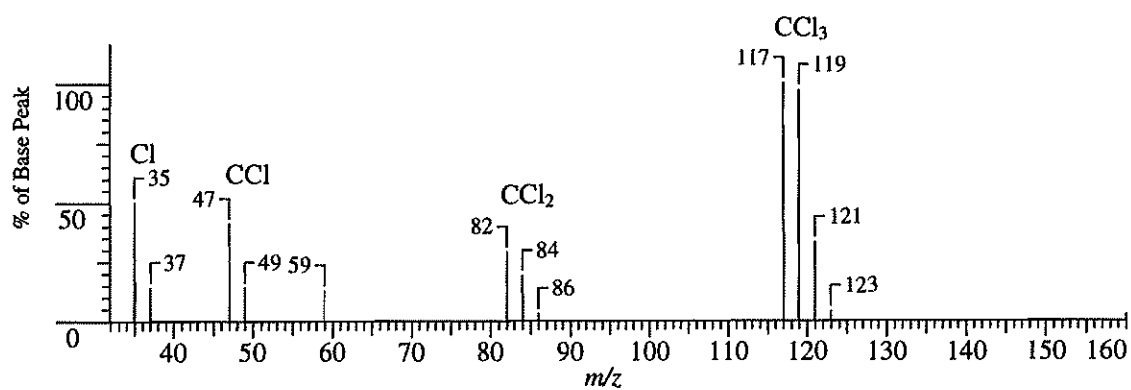
- 4) What are the four important primary regions of the IR spectrum that are helpful in structural elucidation? Explain. (10)

Question B

- 1) What is HDI index? Determine the HDI index of the following compounds. (8)



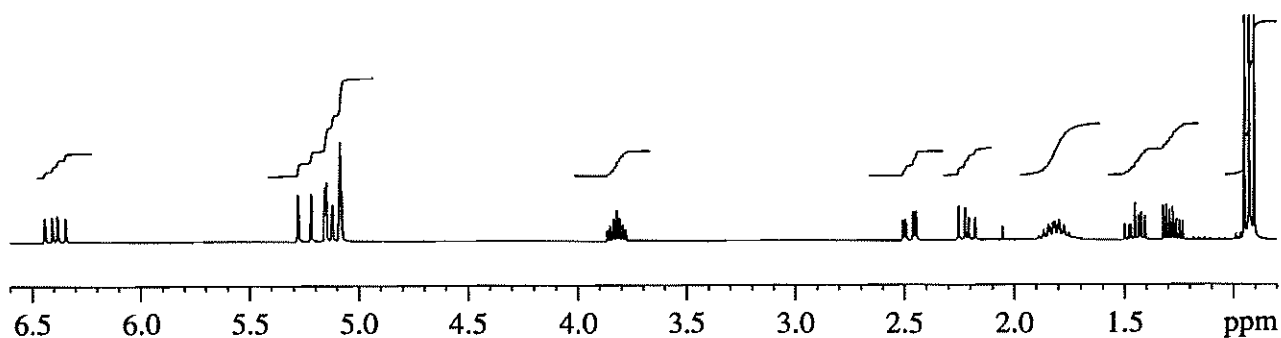
- 2) What information can one extract from the EI spectrum and CI spectra?
(5)



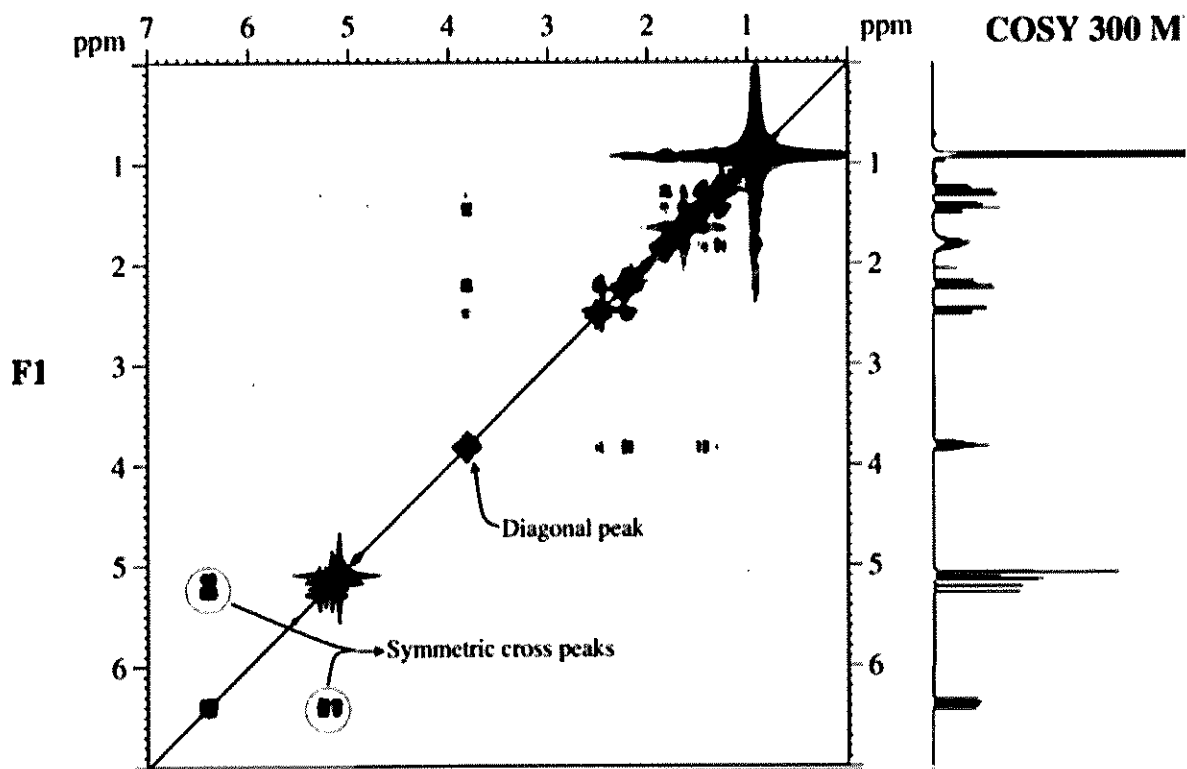
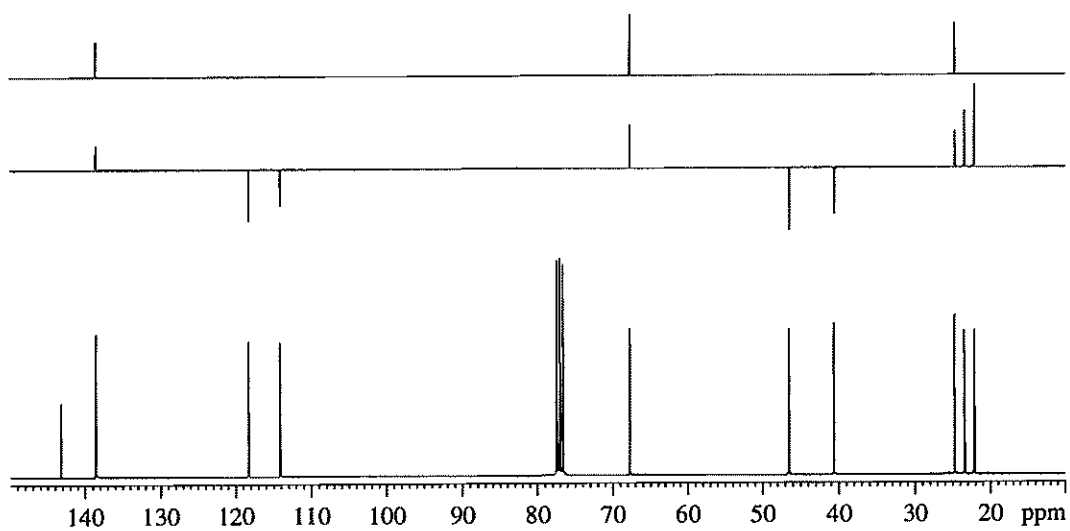
2) Compound A is a molecule with molecular formula $C_{10}H_{18}O$. Determine the molecular structure of compound A from the spectra given below. (12)

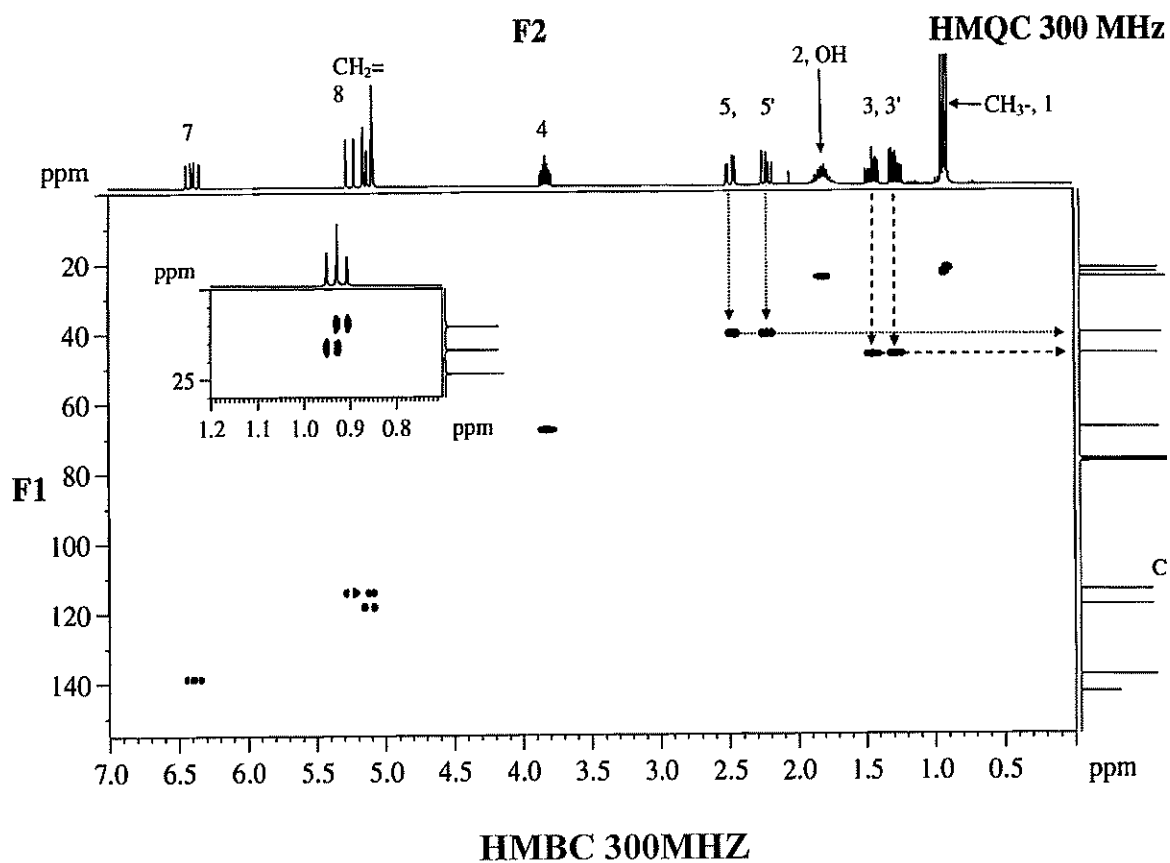
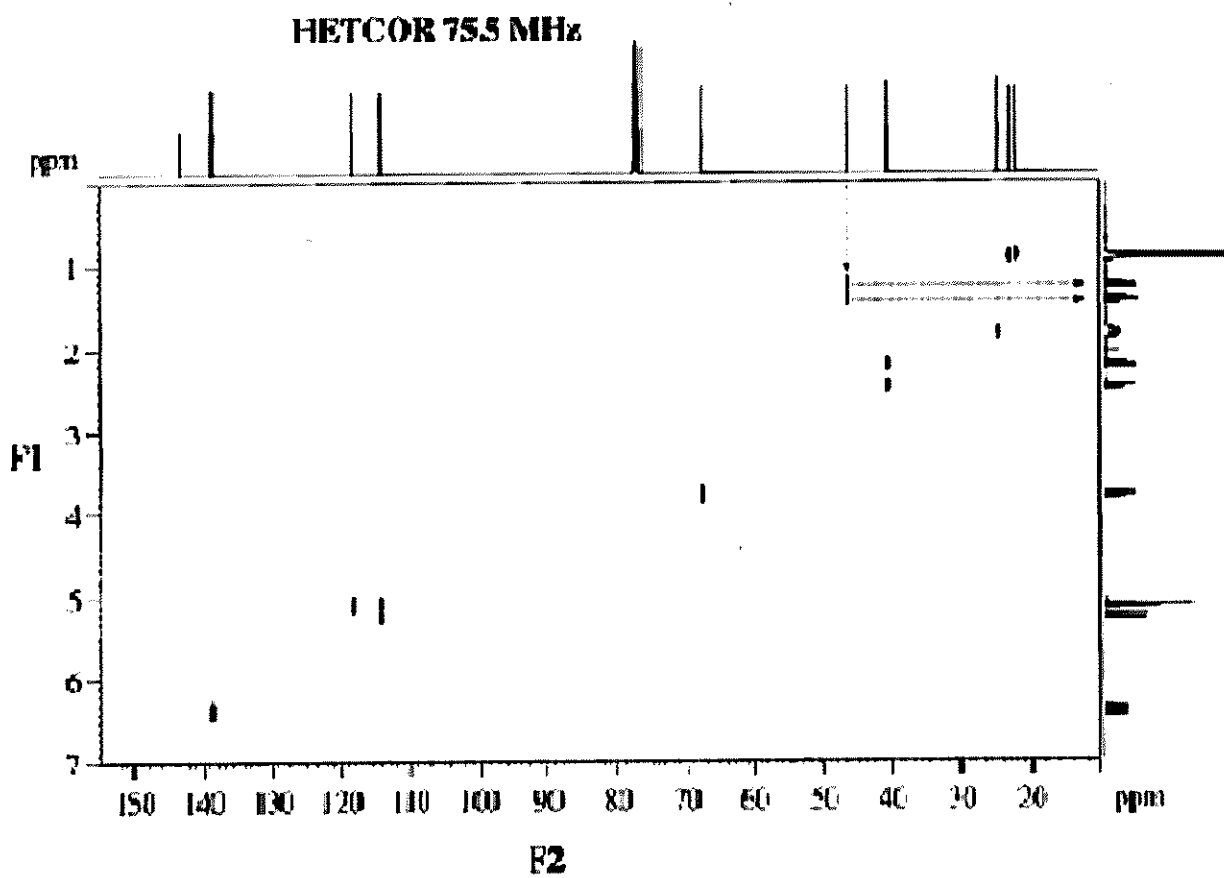
^{13}C , and DEPT experiment spectra of compound A in $CDCl_3$

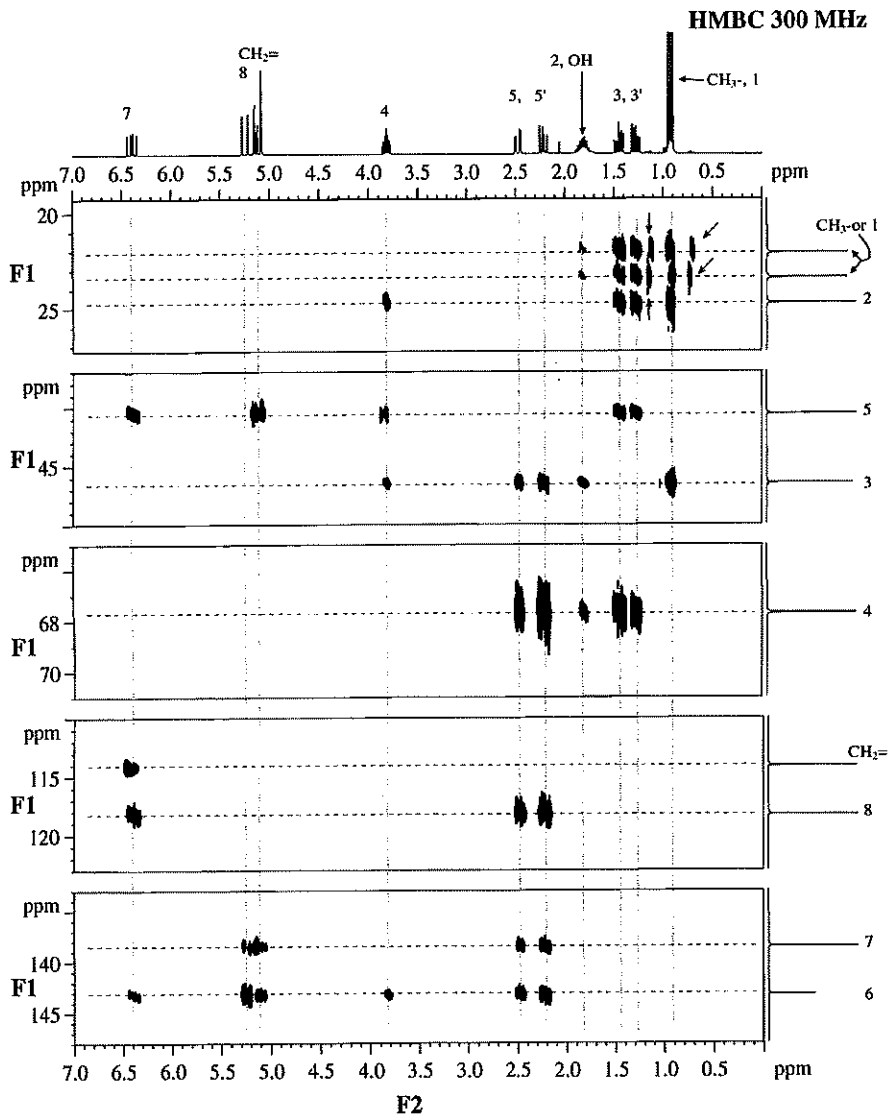
1H NMR 300 MHz



300MHz, 1H

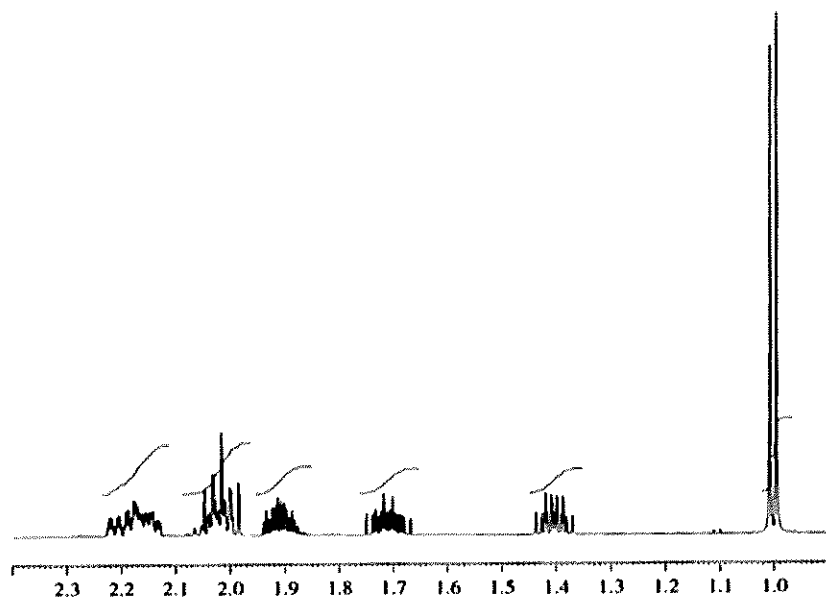
$^{13}\text{C}/\text{DEPT NMR 75.5 MHz}$ 



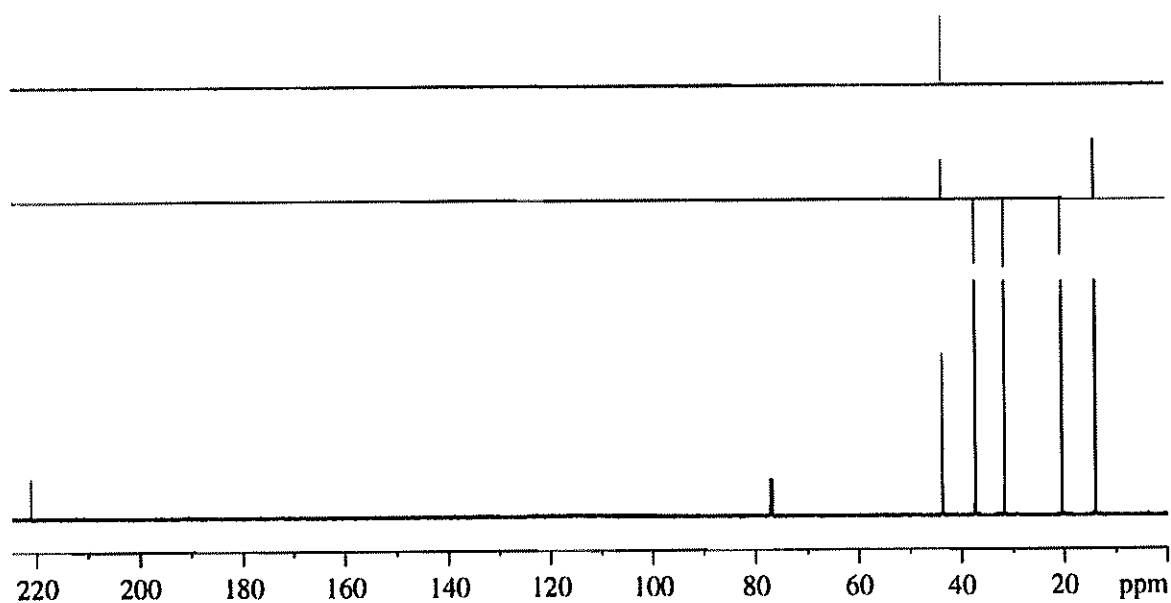


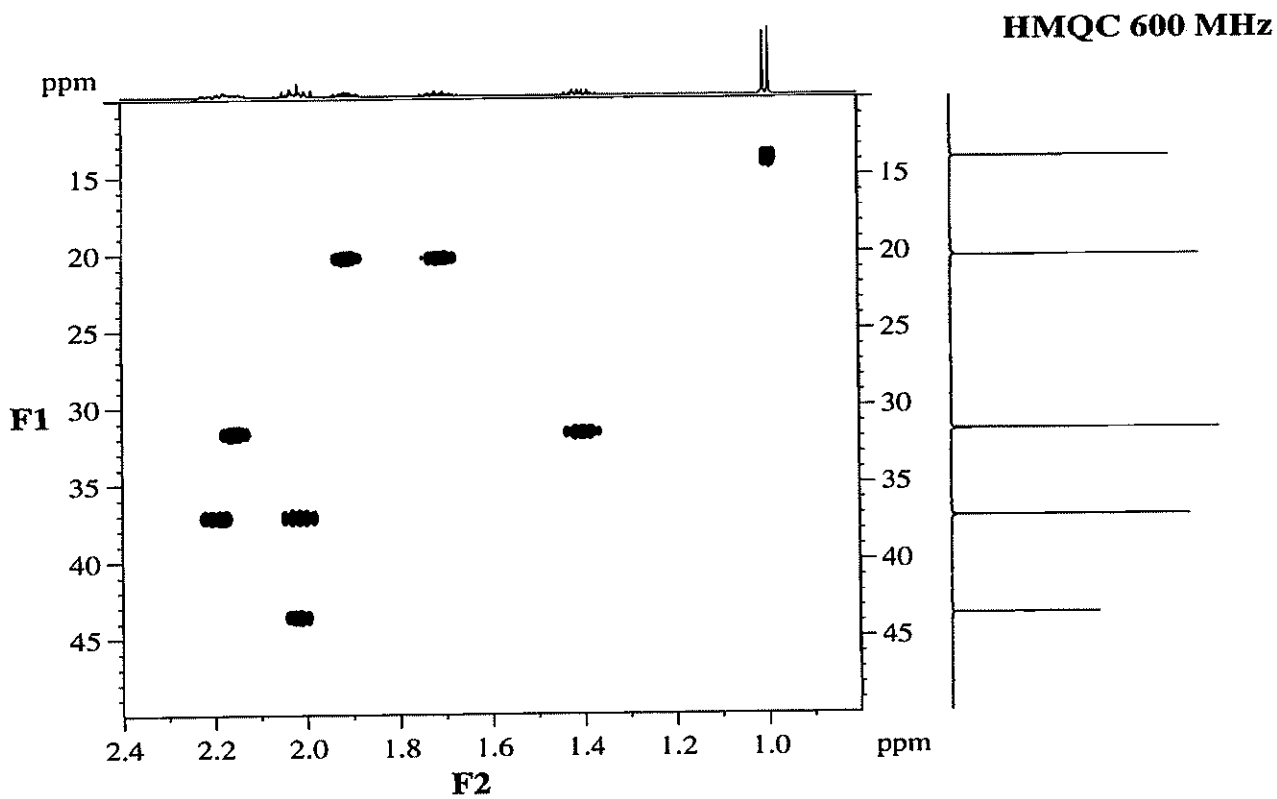
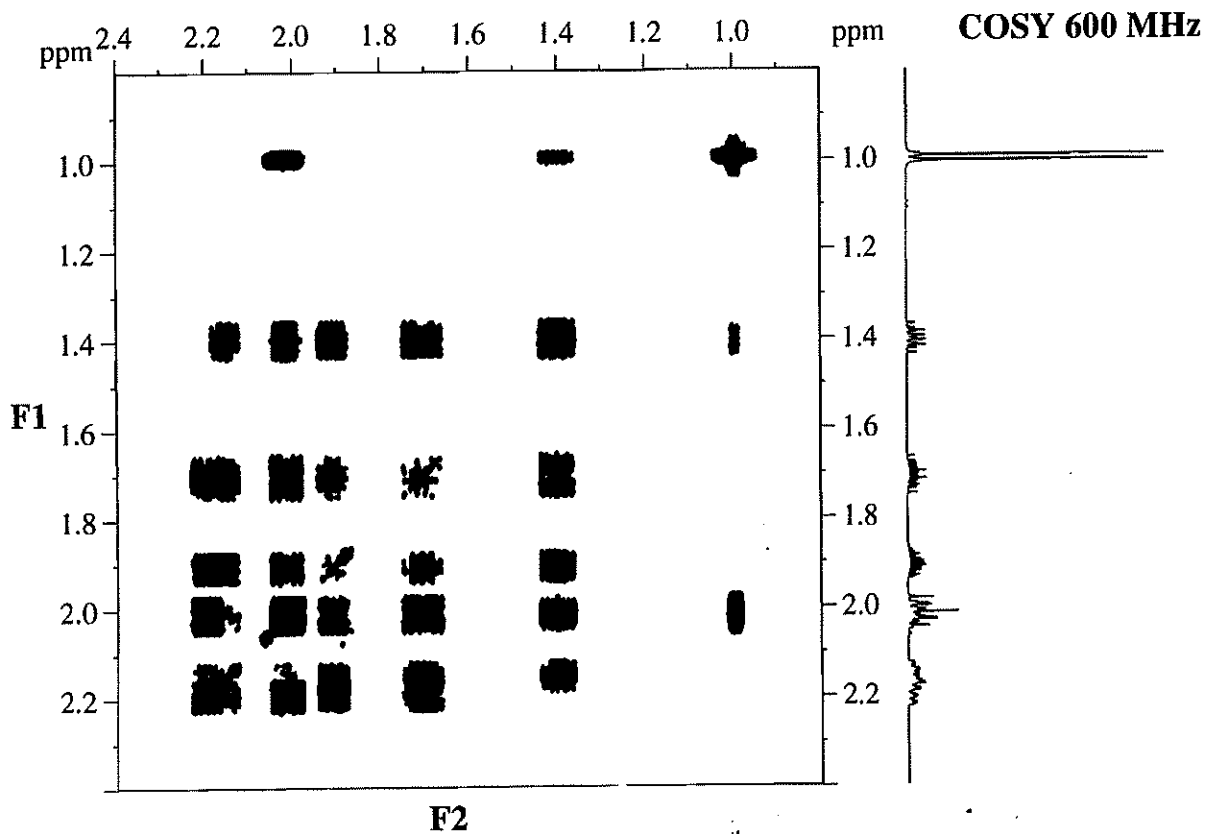
Question C

- 1) Identify the compound $C_6H_{10}O$ from its 1H , ^{13}C /DEPT COSY and HMQC spectra and show correlations. (10)

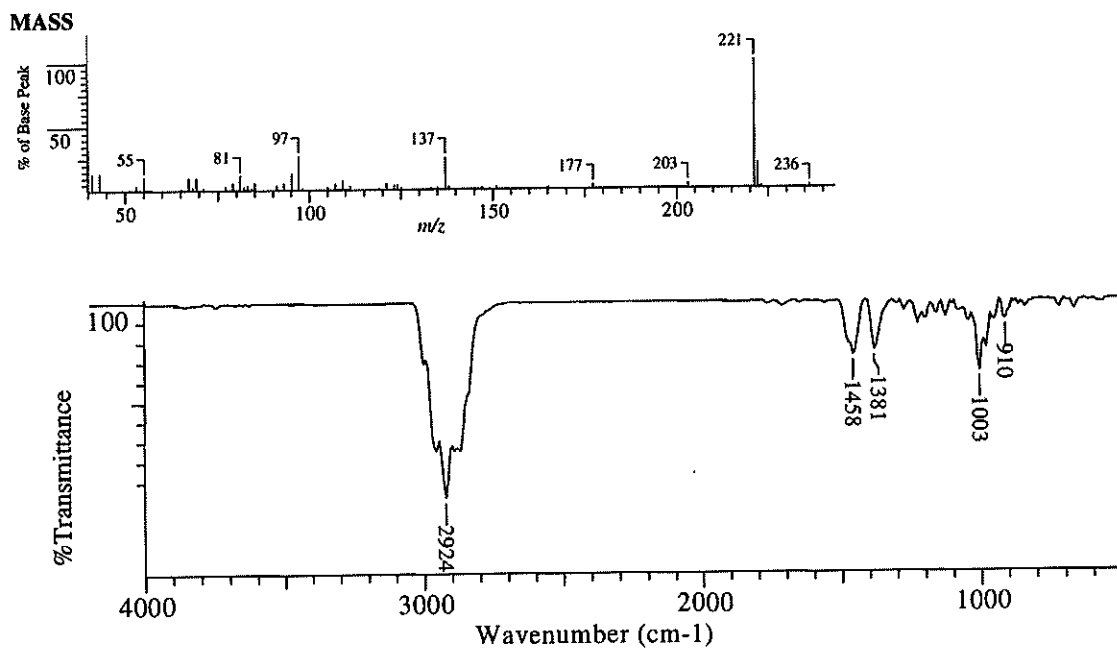


^{13}C /DEPT 150.9 MHz

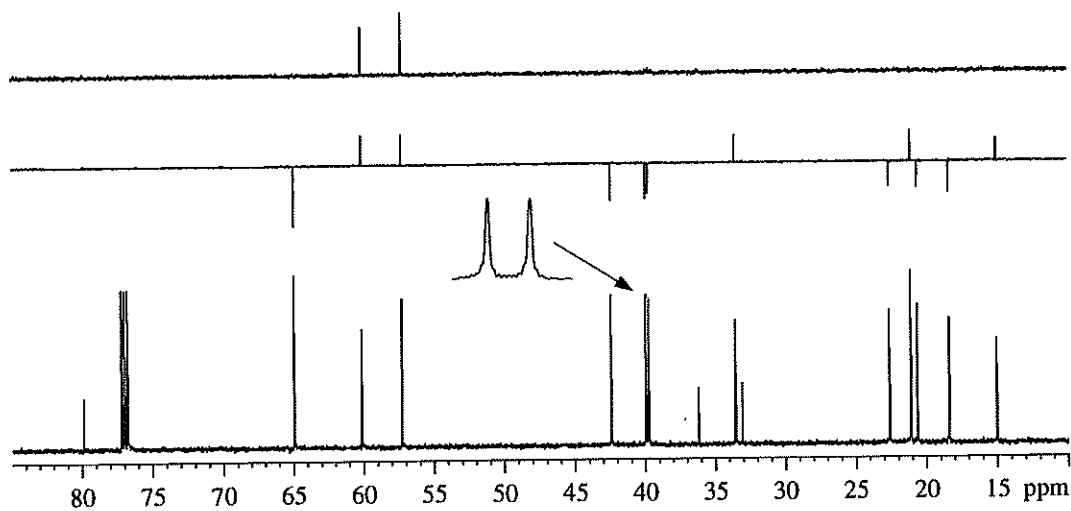


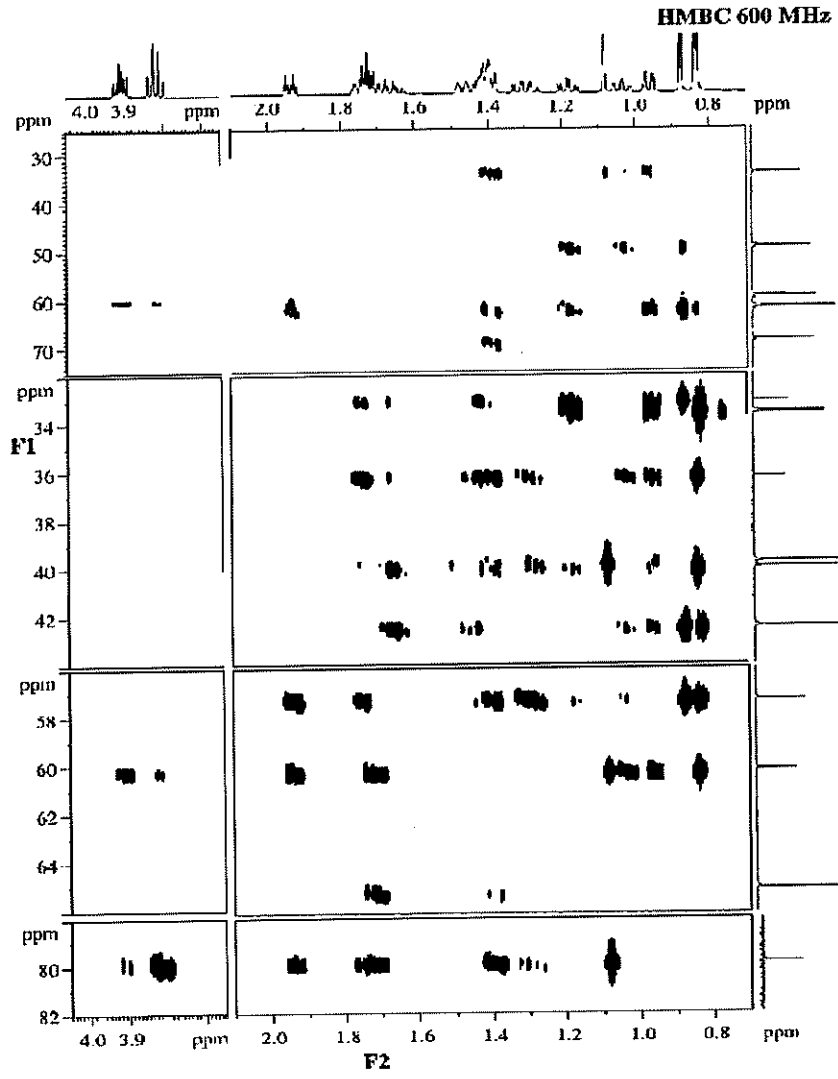


- 2) Determine the structure of the molecule where spectral information Mass, IR, ^1H & ^{13}C DEPT NMR, HMQC and HMBC experiments are given. Assignments need to be convincing and realistic. (15)



$^{13}\text{C}/\text{DEPT NMR 150.9 MHz}$

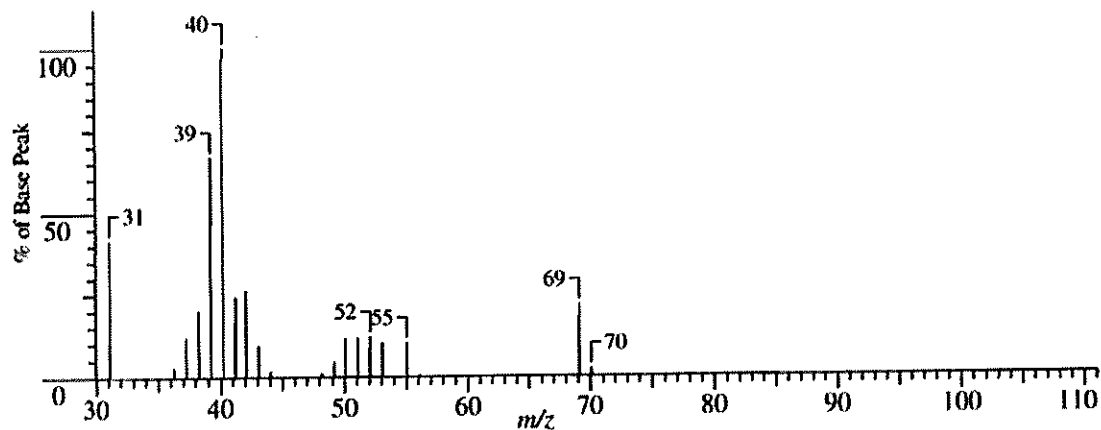




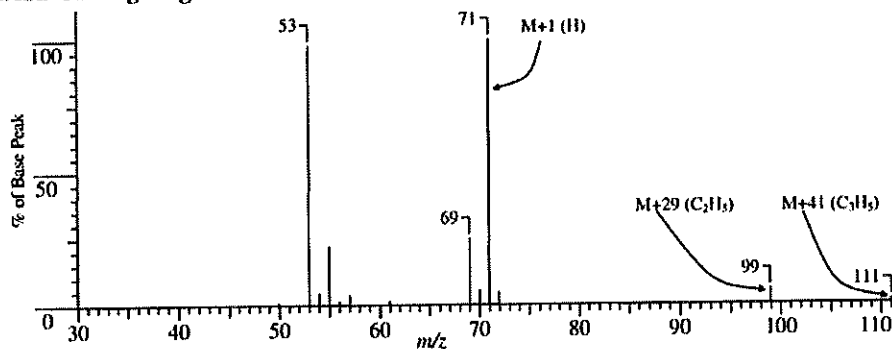
Question D

- 1) Determine the structure of an organic molecule the spectra of which is given. EI, CI, IR, ^1H , ^{13}C /DEPT experiments are given below. (12)

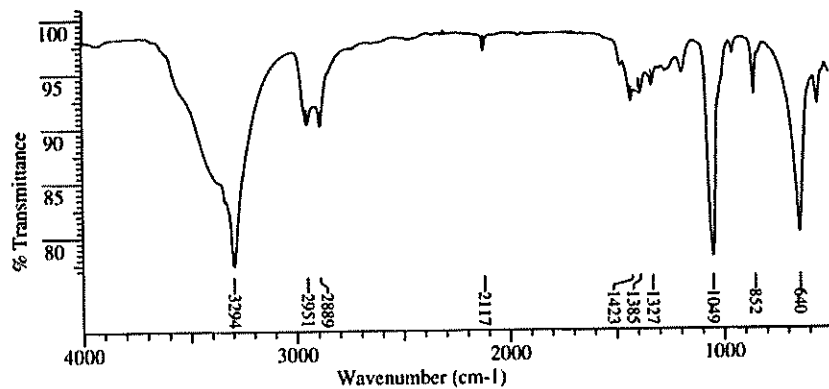
MASS EI

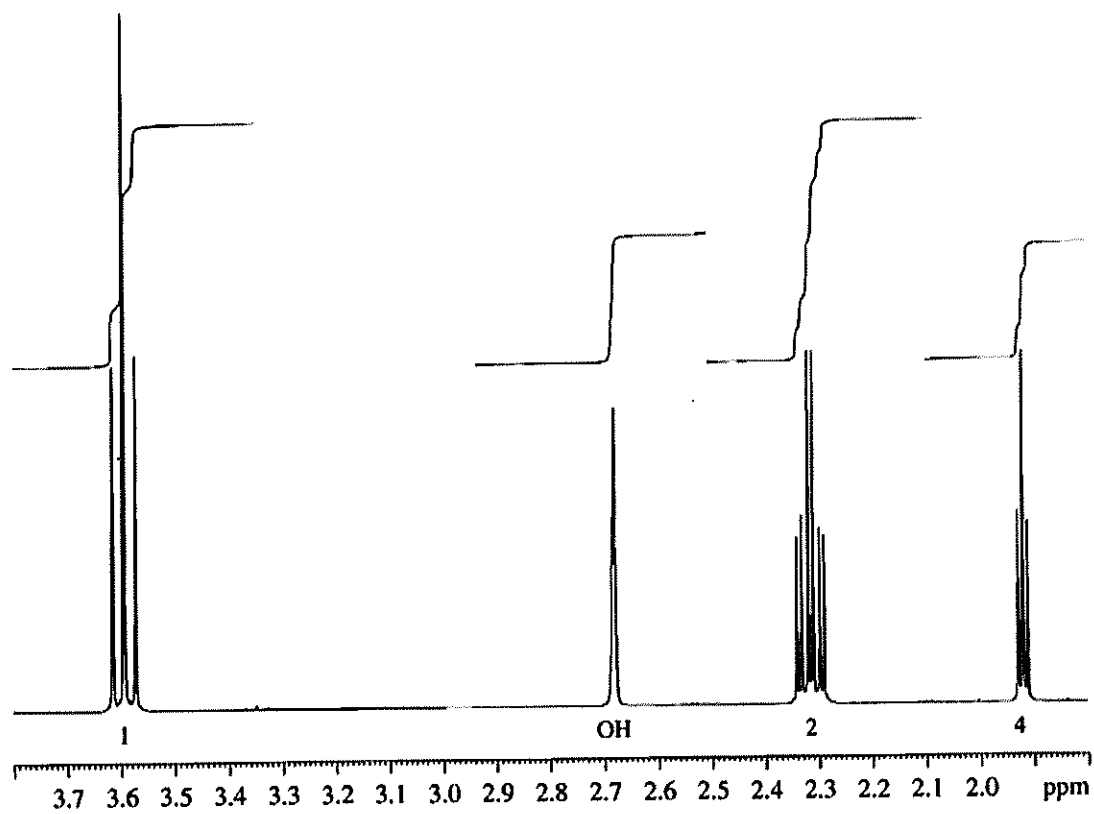


MASS CI reagent gas methane

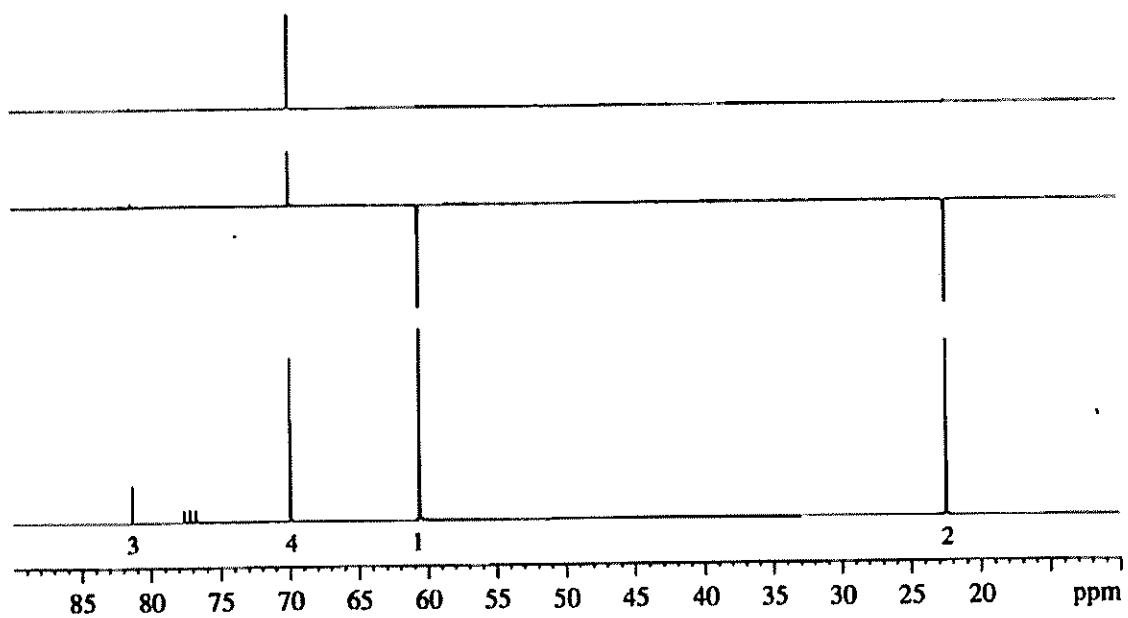


IR

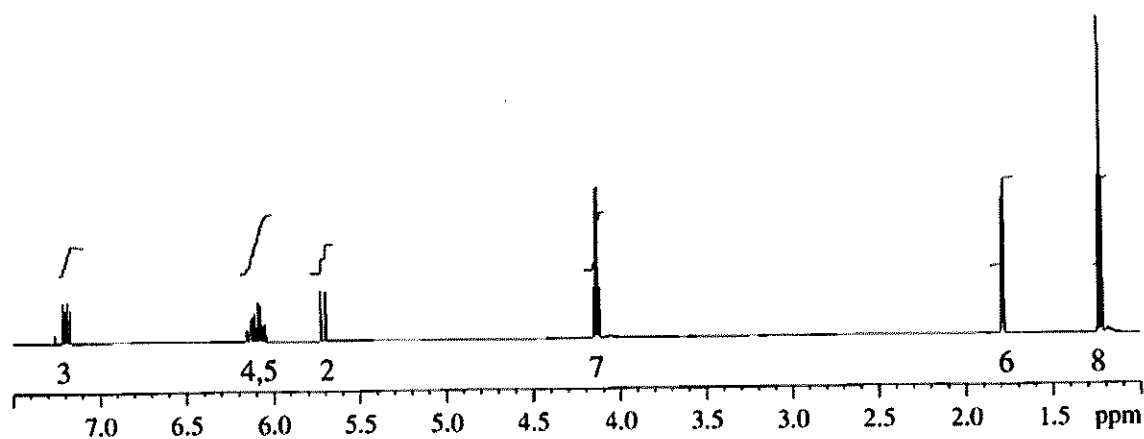
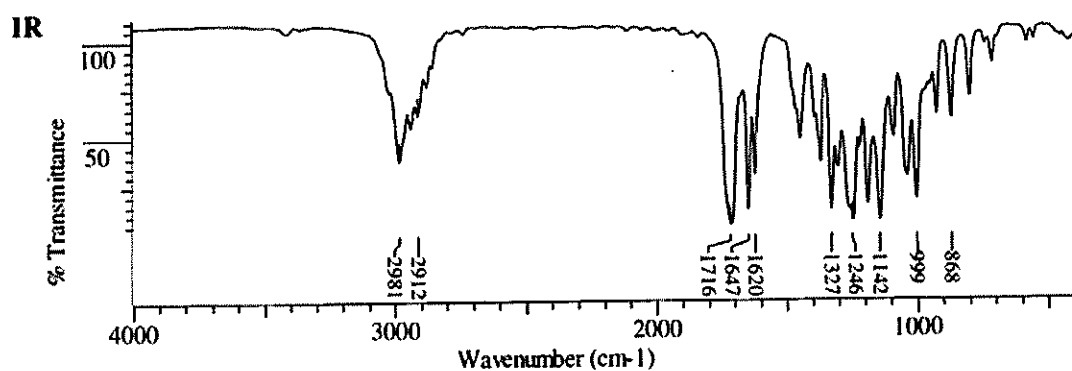
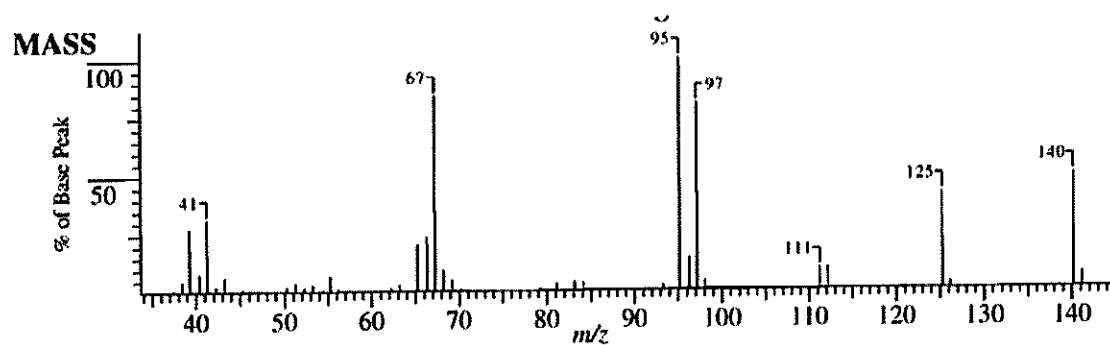


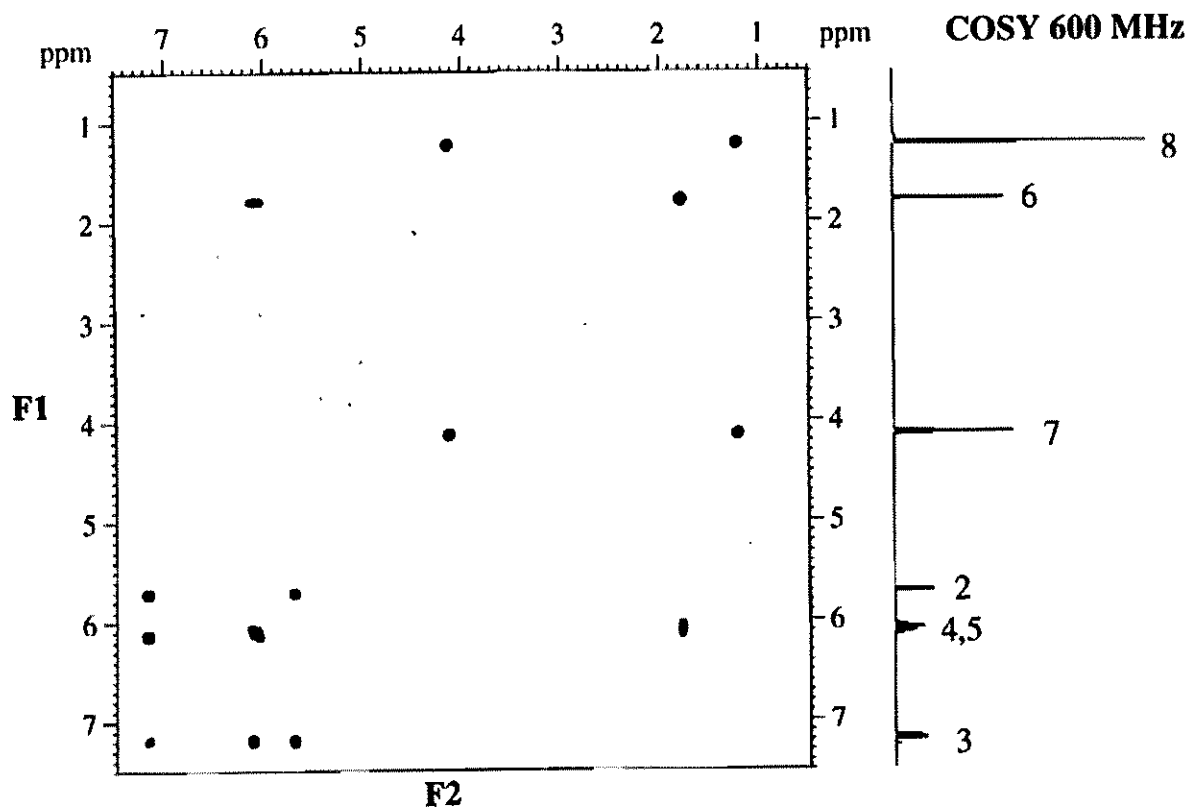
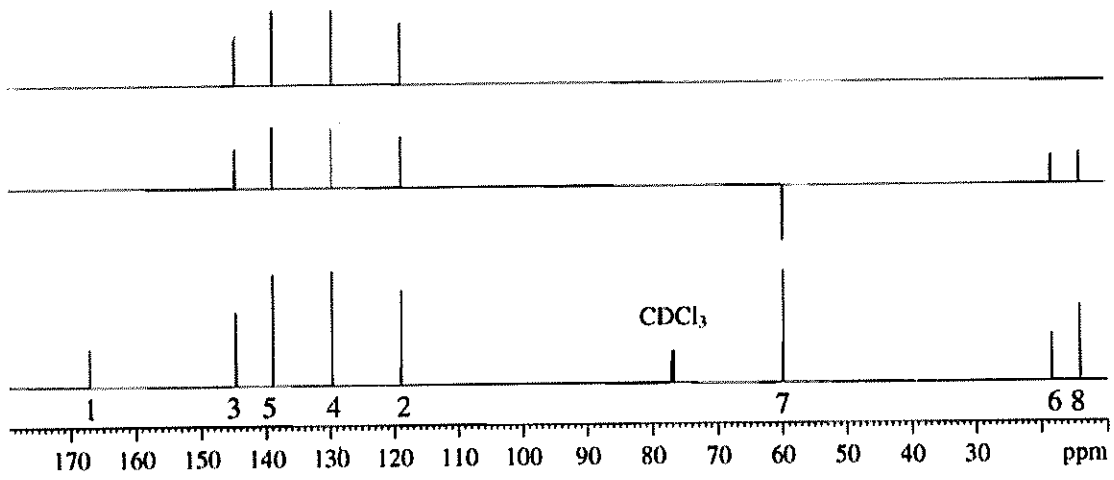


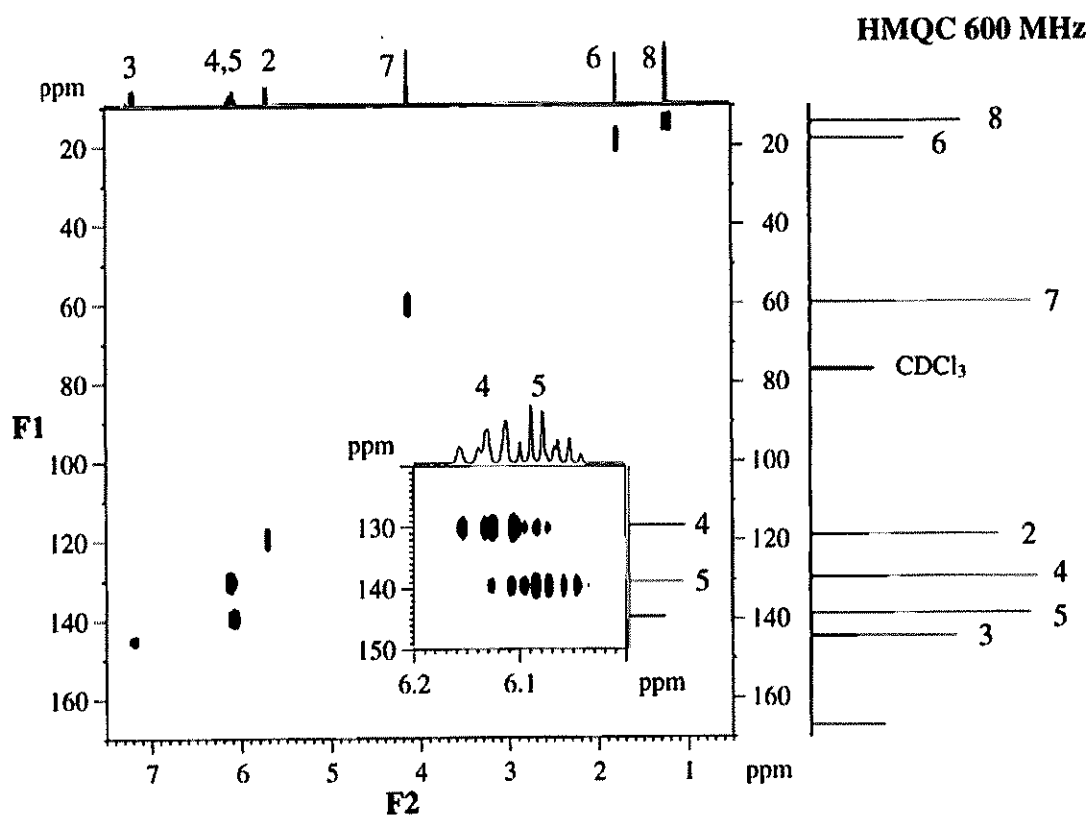
$^{13}\text{C}/\text{DEPT}$ NMR 150.9 MHz



- 2) Determine the structure of an organic molecule the spectra of which is given. EI, IR, ^1H , $^{13}\text{C}/\text{DEPT}$, COSY and HMQC experiments are given below. (13)

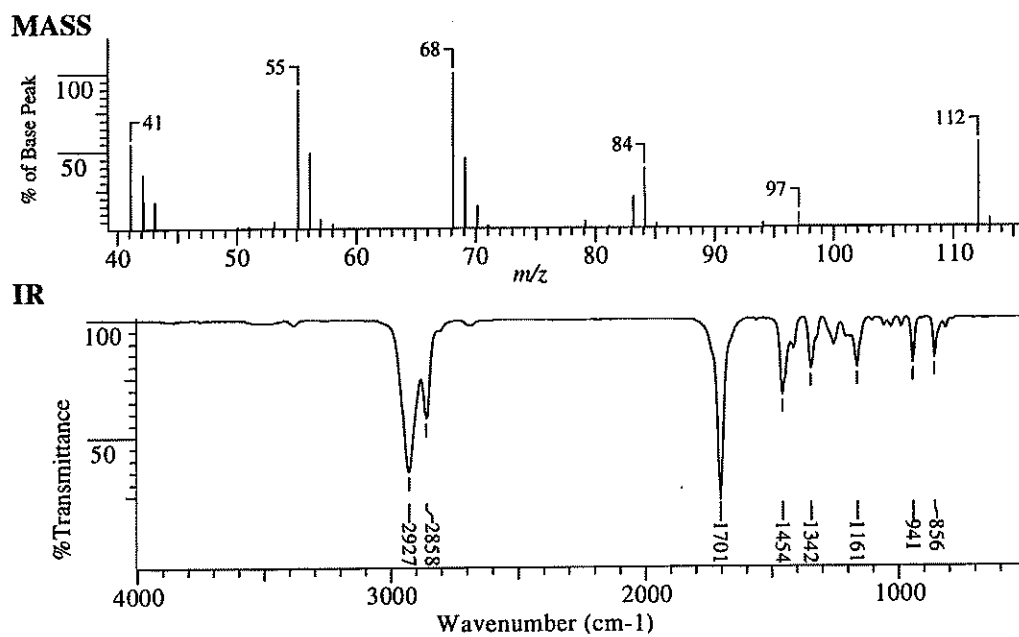


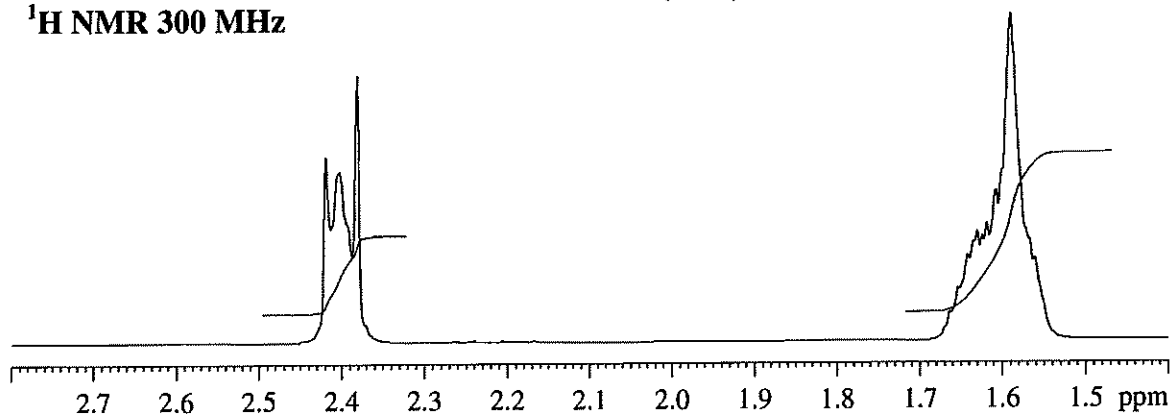
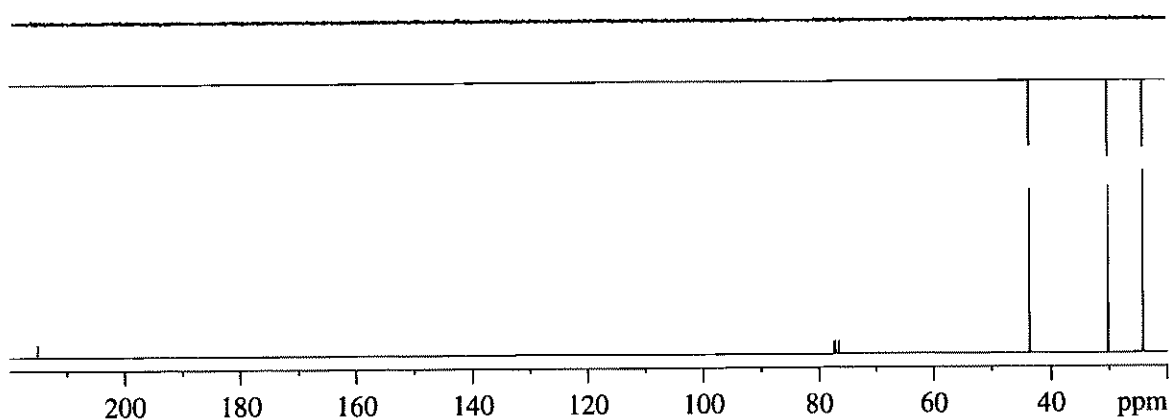
$^{13}\text{C}/\text{DEPT}$ NMR 150.9 MHz



Question E

Determine the structure of the molecule where spectral information Mass, IR, ^1H NMR, and ^{13}C /DEPT is given below. Give explanations in using the information below.



^1H NMR 300 MHz **$^{13}\text{C}/\text{DEPT}$ NMR 75.5 MHz****Question F**

- Compare the contribution of the ^{13}C NMR DEPT experiment and ^1H NMR in structural elucidation of organic molecules. Is one a replacement of the other? (10)
- Benzylic and allylic carbocations are more stable than secondary and methyl carbocations. Do you think these carbocations are more shielded or less shielded? Why? (5)
- What does 2D NMR improve from 1D NMR in structural elucidation of organic molecules? Explain.. (10)