

UNIVERSITY OF ESWATINI

Final Exam – 2019

TITLE OF PAPER : Applied Spectroscopy

COURSE NUMBER : CHE 602

TIME : Three Hours

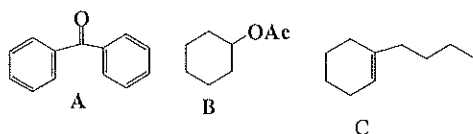
INSTRUCTIONS:

Answer any four (4) questions of the six (6) questions and every question holds 25 marks.

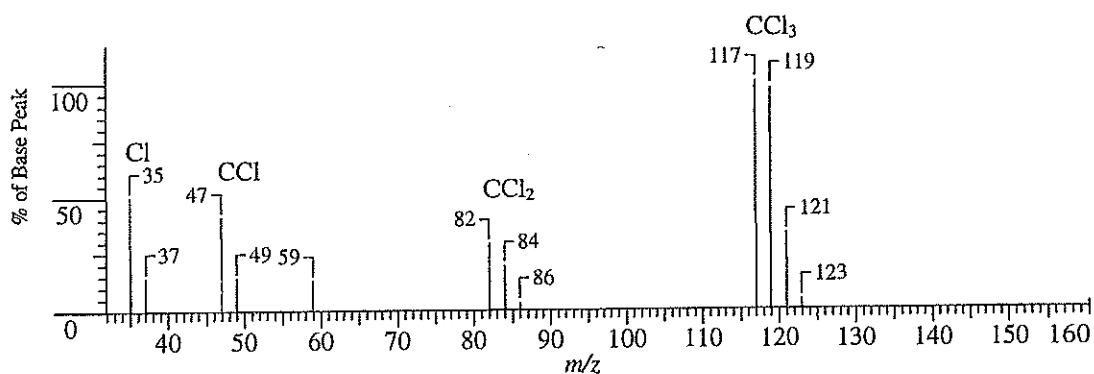
NB: all questions are to be answered in a separate answer sheet.

Question 1

- a) Determine the index of hydrogen deficiency for the following compounds and explain its use in structure determination. (5)

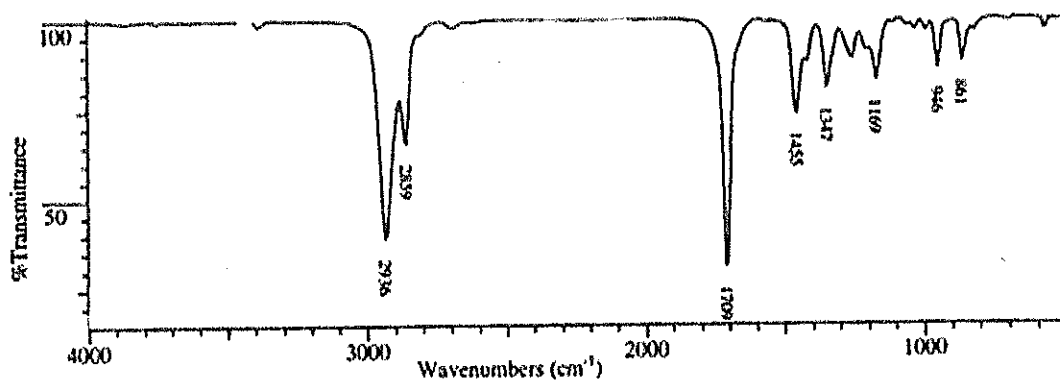


- b) Mention and explain six of the general rules normally applied to predict the prominent peaks in EI spectra using the standard concepts in physical organic chemistry. (10)
- c) Explain and give an example of McLafferty rearrangement. What should a molecule possess to undergo McLafferty Rearrangement? (5)
- d) Define EI in full. What information can one extract from the EI spectrum below and what is the possible structure of the molecule? (5)



Question 2

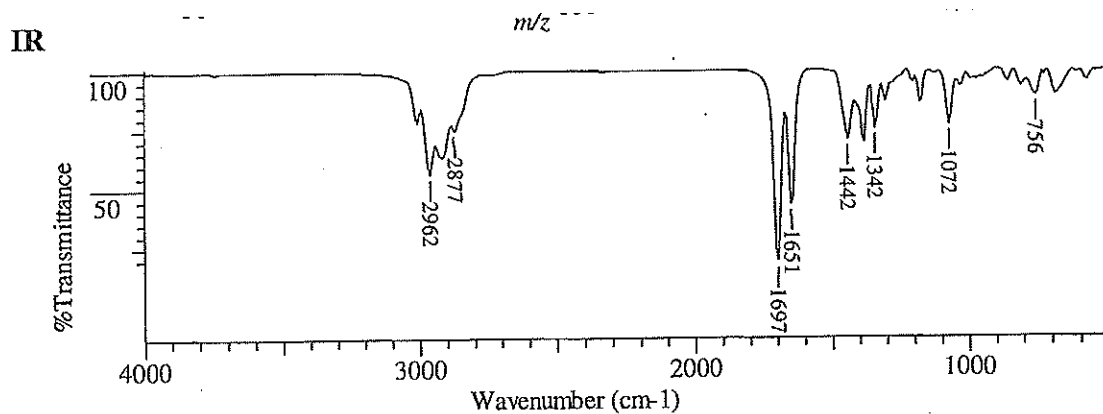
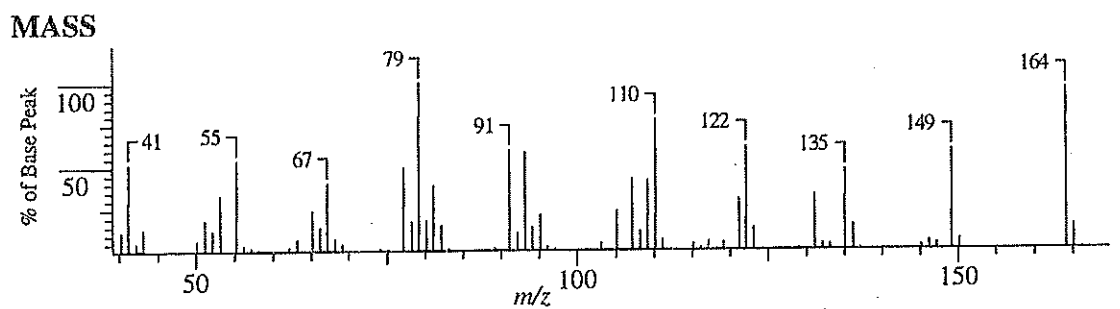
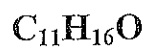
- a) What is the importance of IR spectroscopy in the structural elucidation of organic molecules? (8)
- b) Determine the possible structural information of the compound below from the IR spectrum. (7)



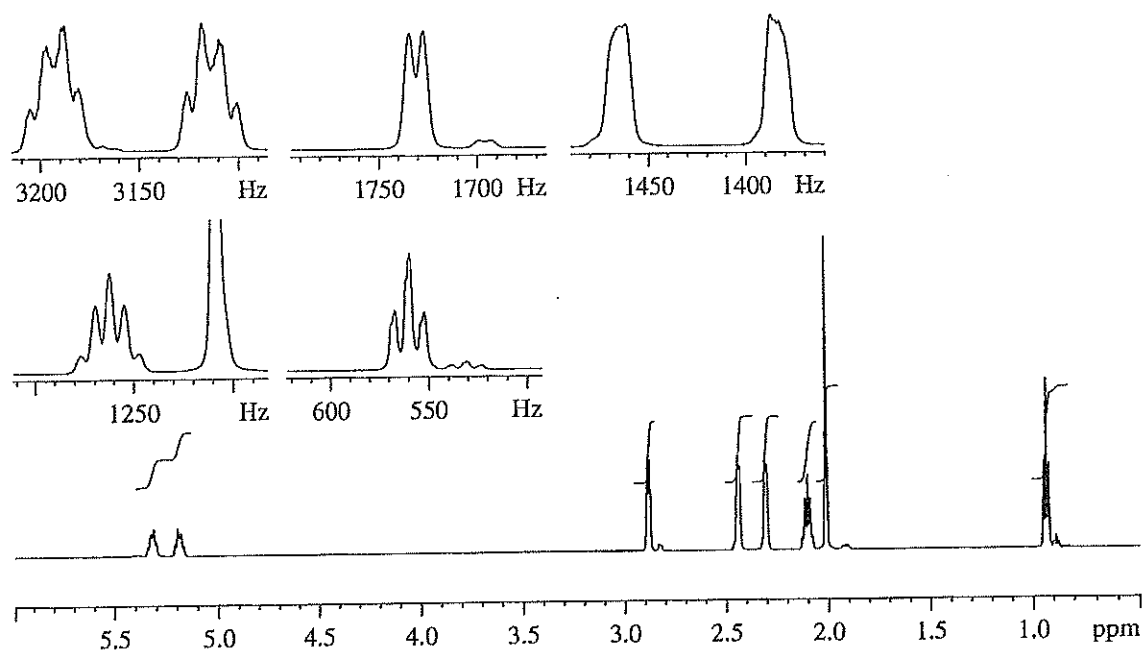
- e) What are the requirements that must be met before attempting interpreting an IR Spectrum?
(9)

Question 3

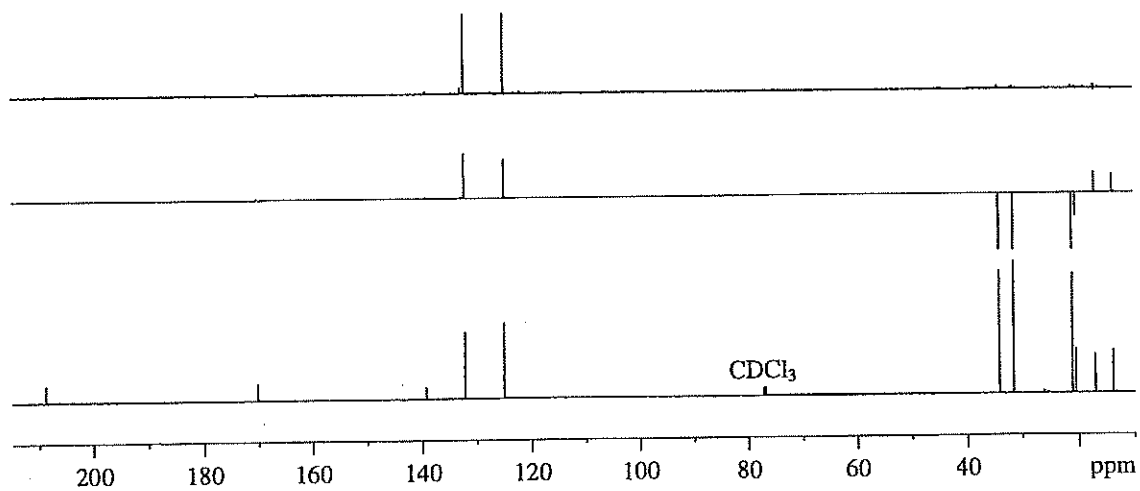
Determine the molecular structure of the compound whose mass spectra is given and the molecular formula is $C_{11}H_{16}O$ IR spectrum, H^1 and ^{13}C /DEPT, HMQC and HMBC experiments are given bellow.



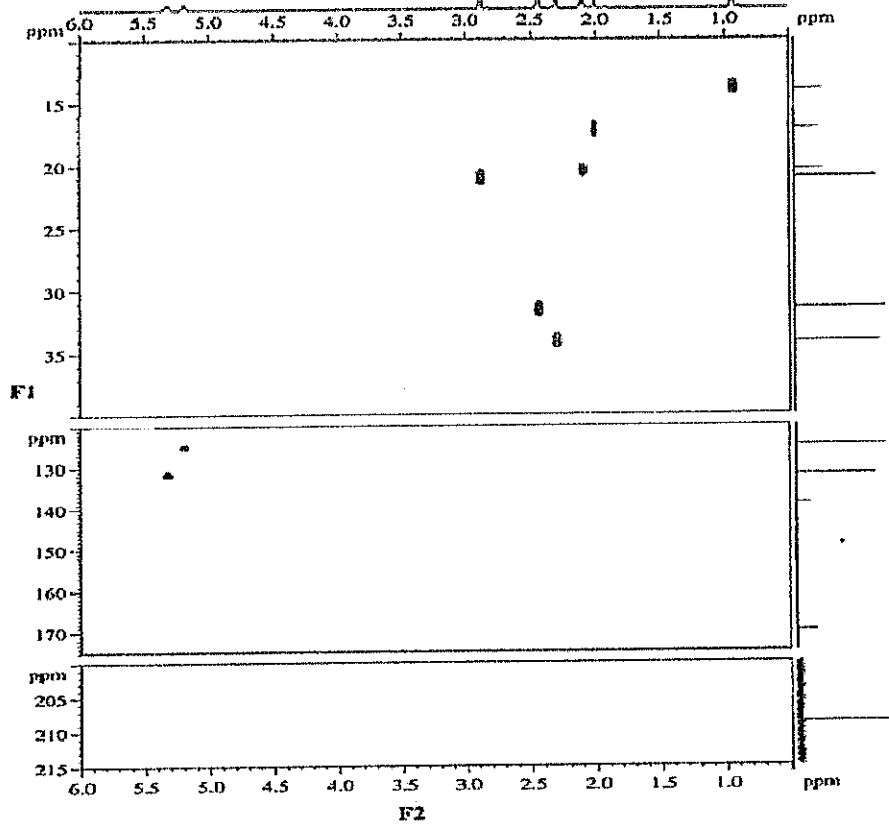
¹H NMR 600 MHz



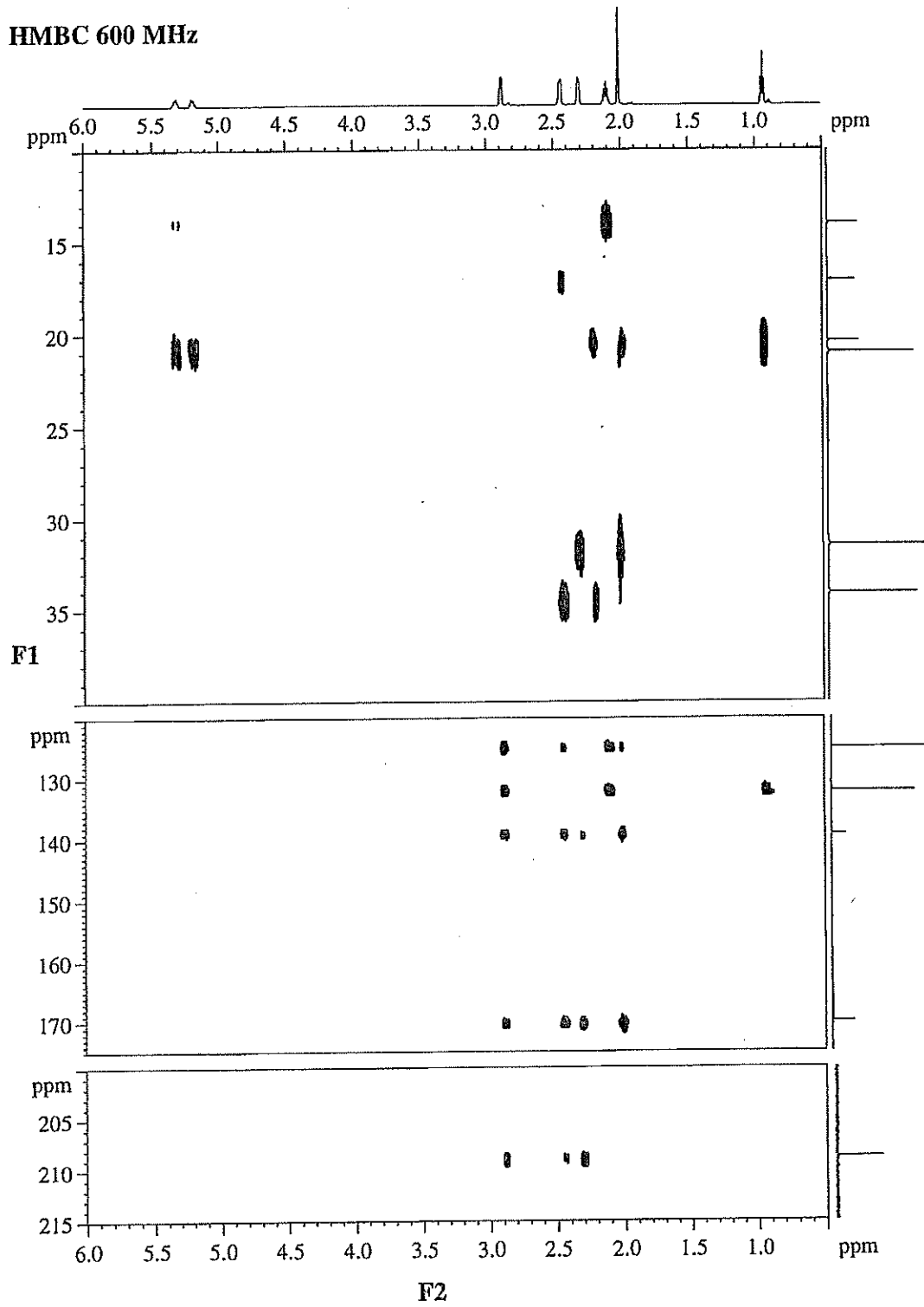
¹³C/DEPT NMR 150.9 MHz



HMQC 600 MHz



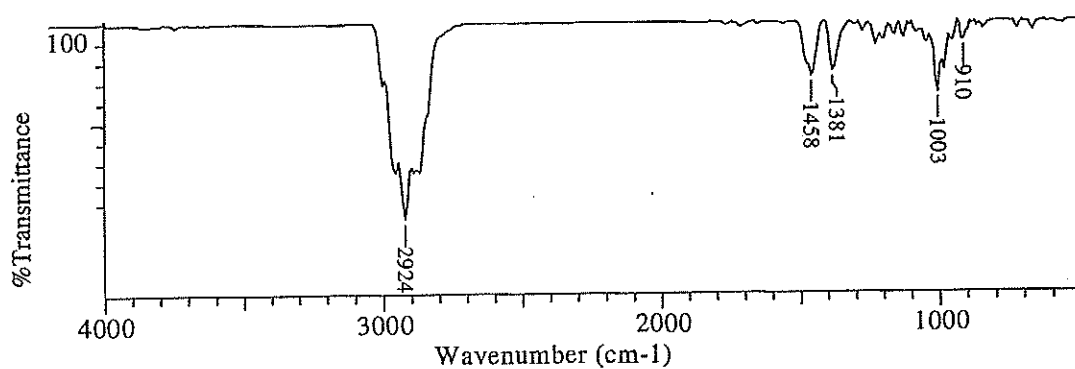
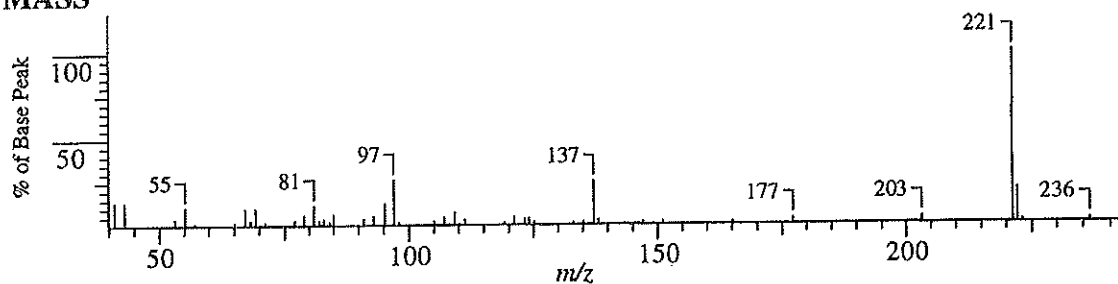
HMBC 600 MHz



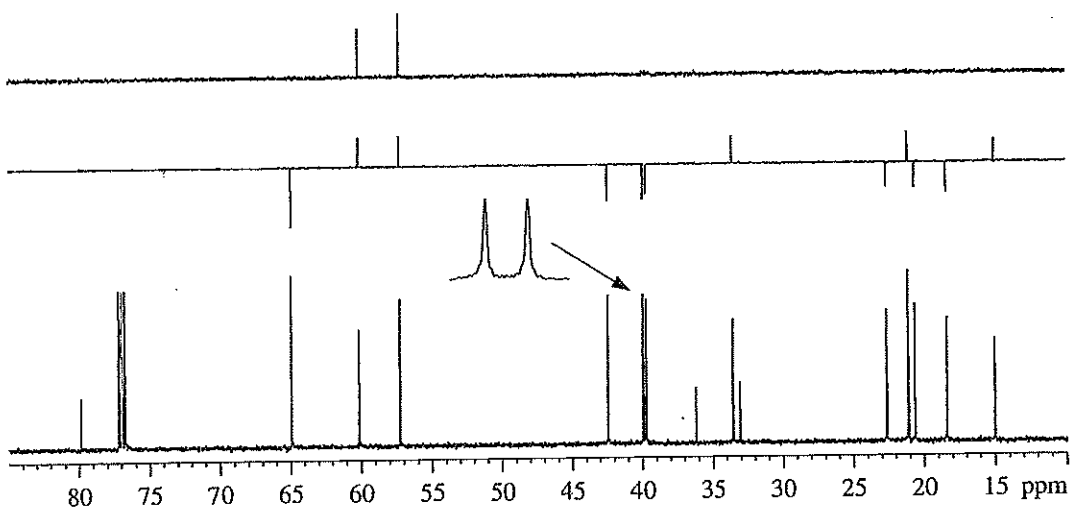
Question 4

Determine the structure of the compound whose information is given below.

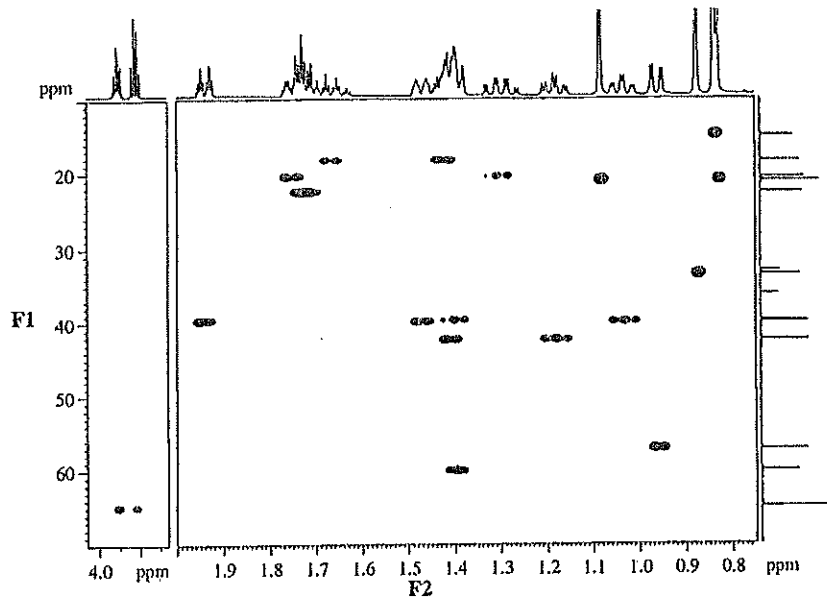
MASS



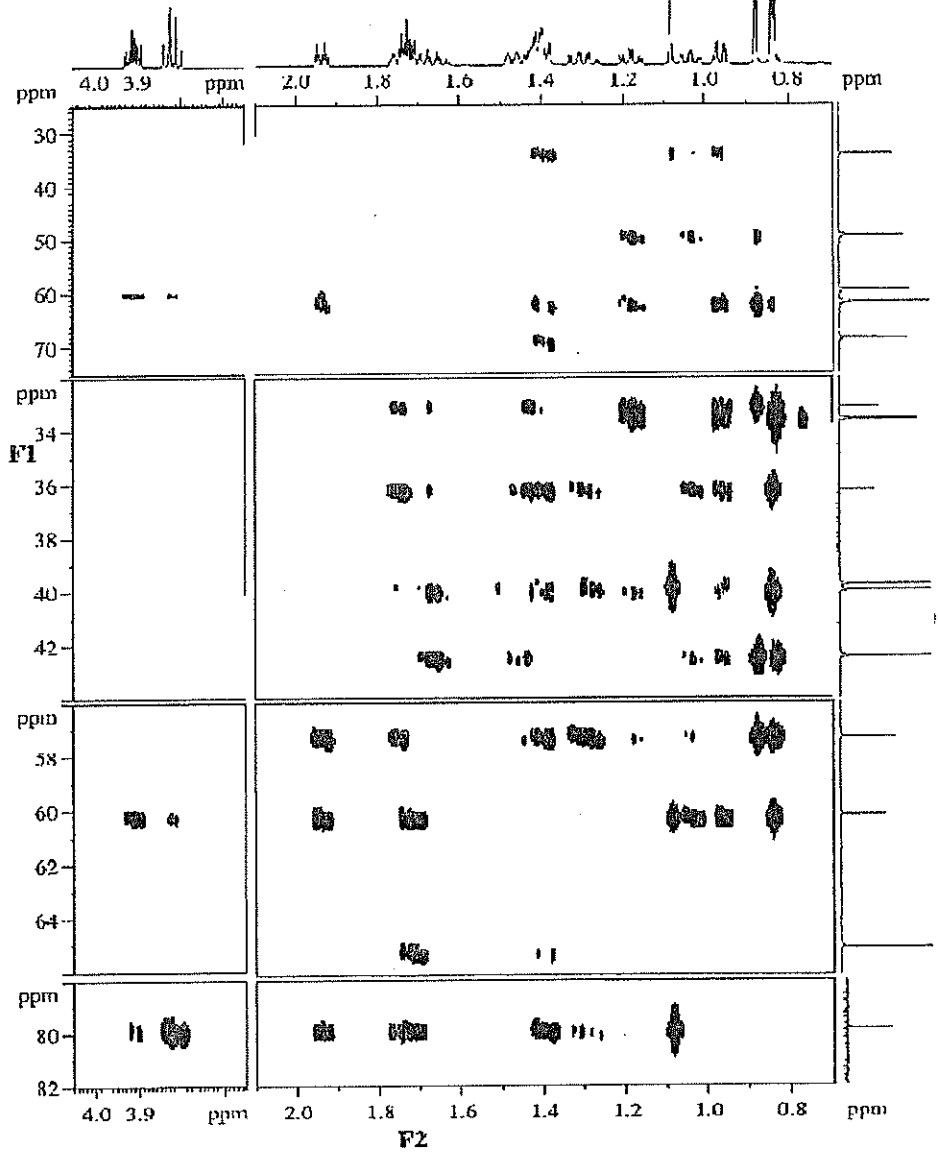
¹³C/DEPT NMR 150.9 MHz



HMQC 600 MHz

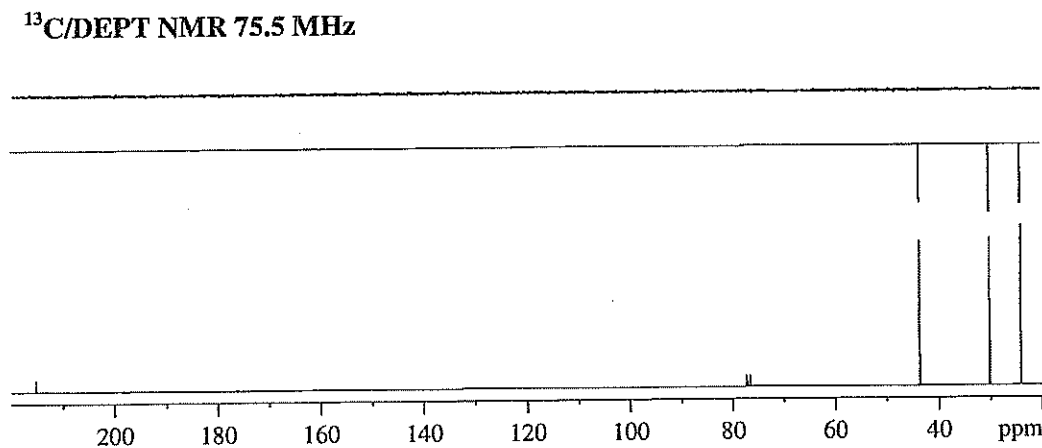
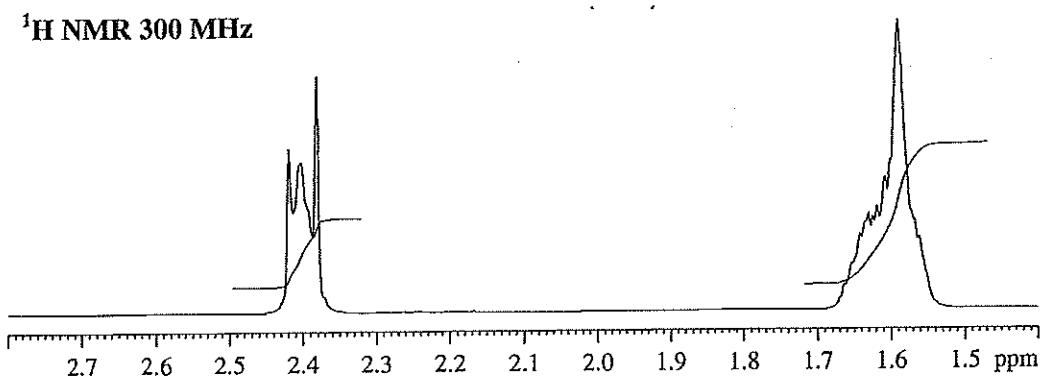
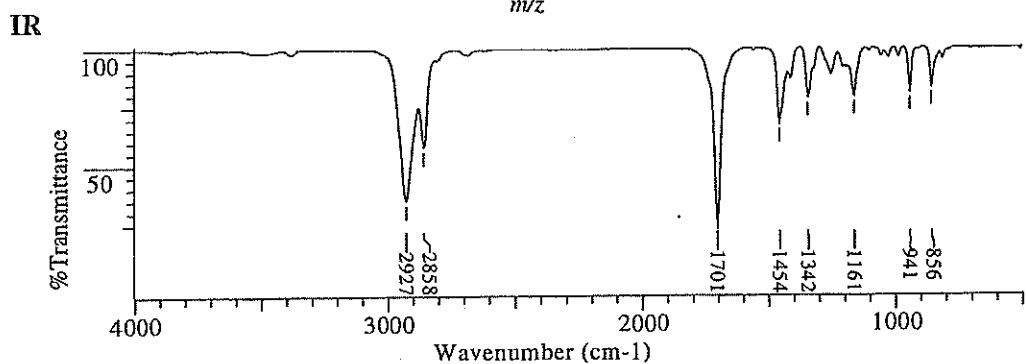
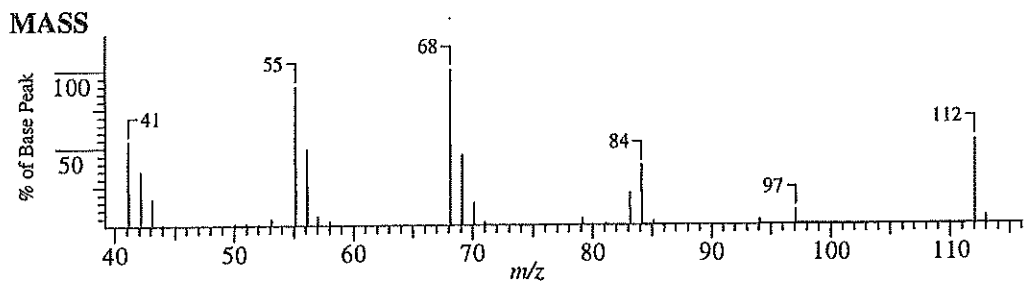


HMBC 600 MHz



Question 5

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



Question 6

- a) Discuss the application of the ^{13}C NMR DEPT experiment in structural elucidation. (10)
- b) 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)
- c) What kind of information do we get from DEPT, HMQC and HMBC experiments? How does it help us for structural elucidation? (10)