



NBU-003-010401

Seat No. _____

M. Sc. (Sem. IV) (CBCS) (All Branches) Examination

April / May - 2017

C-401 Spectroscopy

Faculty Code : 003

Subject Code : 010401

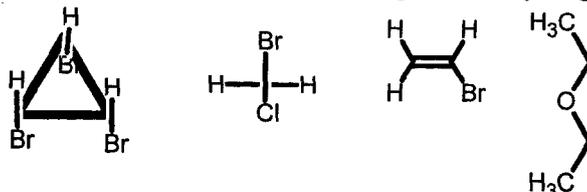
Time : $2\frac{1}{2}$ Hours]

[Total Marks : 70

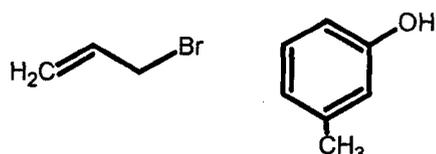
Instruction : All questions carry equal marks.

1 Answer the following (Any seven)

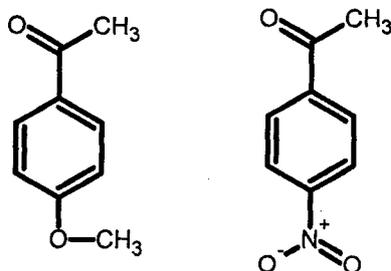
- a. Determine equivalent and non equivalent hydrogen atoms in the following compounds:



- b. How many different types of protons are there in following compounds?



- c. Ethyl acetoacetate shows two carbonyl stretching frequencies. Explain.
d. Which of the following compounds is expected to show a lower C=O stretching frequency? Justify your answer.



- e. Write the full form of TOCSY, INADEQUATE, ROESY and HSQC.
f. What is the most characteristic feature of compounds containing bromine atom in mass spectrometry? Do fluorine and iodine containing compounds show the same feature in their mass spectra?

- g. Why vapour of sample introduced at low temperature in mass spectrometer?
- h. Explain the ring rule. Find ring and double bond in $C_2H_5OC_2H_5$ and $C_6H_5CH_3$.
- i. Derive Lambert's –Beer's law.
- j. Discuss types of UV absorption shift.

2. Answer the followings (Any two)

- a. Give the role of mass analyzer in MS. Describe with diagram the functioning of quadrupole and ion trap mass analyzers.
- b. (i) A liquid compound gave a mass spectrum showing a strong molecular ion at $m/z = 156$. The only fragment ion, are seen at $m/z=127$ and 29. Suggest a structure for this compound.
(ii) While running a new reaction a chemist notices the evolution of a gas. A sample of this gas gave mass spectra in which molecular ion ($m/z=44$) was the largest ion peak The only other significant peaks were obtained at $m/z=28$ and 16. What is this gas?
- c. (i) Draw the hypothetical mass spectrum. Explain M^+ and M^{+} ions, base peak and metastable peak with suitable example.
(ii) What is ionization technique? Explain EI, CI and FAB techniques with their merits and demerits.

3. Answer the following

- a. Sketch the 1H NMR spectrum of butanal and assign each of the protons with multiplicity and coupling constants.
- b. From the given spectral data of a compound with M.F.: $C_8H_{11}N$: IR: 3400 (Sharp), 3000,1600,1500,1400,750,700 cm^{-1} , 1H NMR, ppm: 6-5-7.5(m, 5H), 1.2(t, 3H), 3.1 (q, 2H), 3.3 (s, 1H);MS: 121 (M^+), 106 (BP), establish the structure and also predict the number of ^{13}C NMR signals.

OR

3. Answer the following

- a. A compound of MF C_7H_8O gave IR absorption peaks at 3330.6, 3030.45, 1453.5, 1208.7, 1079.7, 1022.5, 735.2, 697.3, 595. Identify the compound. Also predict 1H NMR and ^{13}C NMR signals.
- b. Draw the hypothetical 1H NMR of ethyl acetate and assign each proton peak with multiplicity and coupling constant.

4. Answer the following (Any three)

- a. Give the application of UV spectroscopy.
- b. Calculate ^{13}C NMR chemical shifts for 3-methyl pentane and 3-hydroxy pentane.
- c. Enlist the technique used in 2DNMR and explain interpretation of any one.
- d. Distinguish following isomeric compounds by IR spectroscopy:
 - (i) $CH_3CH_2C = CH$ and $CH_3-C = C-CH_3$
 - (ii) CH_3-CH_2-OH and CH_3-O-CH_3

5. Answer the following (Any two)

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- a. State the advantage of ^{13}C NMR over a ^1H NMR.
 - b. What is popple notation? Explain AMX spin system with suitable example in briefly.
 - c. Enlist the technique used to simplify the complex system and discuss deuterium labeling techniques with suitable example.
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