UUCMS. No.

B.M.S. COLLEGE FOR WOMEN
BENGALURU -560004

III SEMESTER END EXAMINATION – APRIL - 2024

M.Sc. CHEMISTRY-ORGANIC SPECTROSCOPY
(CBCS Scheme – F+R)

Course Code: MCH303T　　　　　　　　　　　　　　　**QP Code: 13008**
Duration: 3 Hours　　　　　　　　　　　　　　　　　　**Max. Marks:70**

Instruction: Answer Question No. 1 and any FIVE of the remaining.

1. Answer any *TEN* questions　　　　　　　　　　　　　　　　**(2×10 =20)**

a) Aniline absorbs at 280 nm but in acidic solution, the main absorption band is seen at 203 nm which is comparable to benzene. Explain

b) Define bathochromic shift with an example?

c) List out the modes of vibrations of CO_2 in IR Spectroscopy

d) Mention the reference compound used in NMR. List out its advantages.

e) Calculate the chemical shift value in ppm for a proton that has resonance 128 Hz downfield from the reference on a spectrometer that operates at 60 MHz

f) How is PMR used to establish on which carbon, monochlorination of methyl ethyl ether occurs?

g) The proton decoupled ^{13}C NMR spectrum of tribromobenzene ($C_6H_3Br_3$) consists of two signals only. Which tribromobenzene is it?

h) What is Karplus relationship? Write the equation

i) Sketch and explain the ^{31}PNMR spectrum of PPh_3.

j) Explain the mass spectra of 1-propanol.

k) EI-MS are recorded only in rarified gaseous state. Explain

l) The mass spectrum of benzene shows a peak at m/z 33.8. Account for the peak.

2. a) Using the Woodward-Fieser rules, calculate the absorption maximum for each of the following compounds:
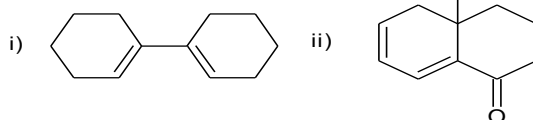
b) How is UV-Visible spectroscopy useful in determining the strength of hydrogen

bonding.

c) Explain Fieser-Kuhn rule for polyenes. **(4+3+3=10)**

3. a) Explain second order splitting taking suitable example.

b) Discuss diamagnetic shielding effect in case of benzene and acetylene. **(5+5=10)**

4. a) Off resonance ^{13}C NMR data for three isomeric alcohols with molecular formula

$C_4H_{10}O$ is given below:

A (δ ppm): 31 (q), 69.5 (s)

B (δ ppm): 11 (q), 22 (q), 31 (t), 69.5 (d)

C (δ ppm): 19 (q), 31 (d), 69.8 (t)

Identify alcohols, assign peak to carbon atoms.

b) Explain the factors affecting chemical shifts of alkyl halides and carbonyl compounds in

^{13}C NMR spectroscopy. **(6+4=10)**

5. a) Discuss evaporative ionization techniques. Give their applications.

b) Illustrate McLafferty's rearrangement with suitable example. **(6+4=10)**

6. a) Discuss the phenomenon of proton exchange by taking ethanol as an example.

b) Write a note on the effect of restricted rotation on proton NMR spectra.

c) Explain relaxation processes in NMR **(4+3+3=10)**

7. a) Write a note on: i) DEPT spectrum   ii) NOE effects

b) An aromatic compound (molecular mass=135) gives the following signals in its ^1H

NMR spectrum: singlet (δ 2.09, 3H), a distorted singlet (δ 3.09,1H) a multiplet

(δ 7.24, 3H), a multiplet (δ 7.75, 2H). Predict the structure of the compound. **(6+4=10)**

8. a) With a neat diagram, explain the instrumentation of a double focused mass

spectrometer.

b) Identify the structure of the compound from the below given data and interpret the data

to the structure obtained. Molecular formula: $C_5H_7NO_2$, ^1H NMR (CDCl$_3$) δ: 4.3 ppm

(quartet, 2H, J = 7.5 Hz), 3.5 ppm(s, 2H), 1.3 ppm (triplet, 3H, J = 7.5 Hz); ^{13}C NMR

(CDCl$_3$) δ: 165, 115, 62, 25, 15 ppm. **(5+5=10)**

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