REV-01
MSC/75/80

2025/05

SET A

M.Sc. CHEMISTRY
FOURTH SEMESTER
APPLICATION OF SPECTROSCOPY-II
MSC – 403

[USE OMR FOR OBJECTIVE PART]

Duration: 1:30 hrs. **Full Marks: 35**

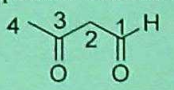
(Objective)

Time: 15 mins. **Marks: 10**

Choose the correct answer from the following: ***1×10=10***

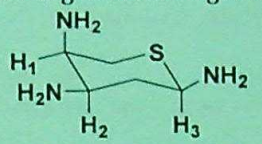
1. The peak of CD2Cl2 in 13C NMR will be
   a. singlet
   b. triplet
   c. quartet
   d. quintet

2. Which carbon of the following compound will show peak in DEPT-90 spectrum



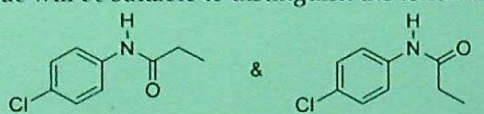
   a. C1
   b. C2
   c. C3
   d. C4

3. Which one is correct for the following molecule regarding its NMR study?



   a. H_1-H_2: COSY & H_2-H_3 NOESY
   b. H_1-H_2: NOESY & H_2-H_3 COESY
   c. H_1-H_3: COSY & H_2-H_3 NOESY
   d. H_1-H_3: NOESY & H_2-H_3 COESY

4. Which NMR technique will be suitable to distinguish the followings



   a. ^{1}H-NMR
   b. DEPT
   c. COSY
   d. NOESY

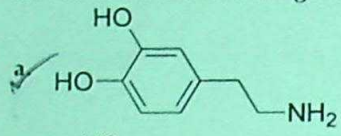
5. If a molecule ($C_xH_yN_z$) shows molecular ion peak in EI-MS m/z = 153.03, a distinct peak at 2250 cm^{-1} in IR and a singlet (δ = 8 ppm, 3H) in ^{1}H-NMR, and DBE = 10, the correct formula will be
   a. $C_9H_5N_3$
   b. $C_9H_4N_2$
   c. C_9H_7N
   d. $C_9H_3N_3$

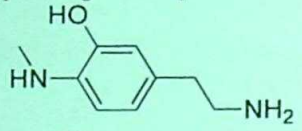
6. The typical energy of an electron beam used in mass spectrometry bear
   a. 15 eV
   b. 70 eV
   c. 55 eV
   d. 25 eV

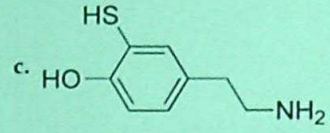
7. In the mass spectrum of methane (CH_4), the molecular ion peak appears at m/z = 16. What would be the base peak if the most abundant fragment is CH_3^+?
   a. m/z = 15
   b. m/z = 14
   c. m/z = 16
   d. m/z = 1

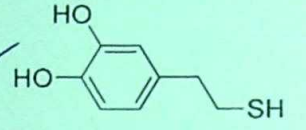
8. The most abundant ion peak observed in mass spectrometry is known as
   a. Molecular ion peak
   b. Base peak
   c. Fragmentation peak
   d. None of the above

9. In mass spectrum of a compound the molecular ion ($M^{\bullet}$) peak is observed at m/z = 153. Which of the following compound is corresponding to the spectrum

a. 

b. 

c. 

d. 

10. For a compound with molecular formula C_2H_6 the M+1 peak in mass spectrum will be found at
   a. m/z = 30
   b. m/z = 32
   c. m/z = 31
   d. m/z = 29

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Descriptive

Time : 1 hr. 15 mins. **Marks: 25**

[Answer question no.1 & any two (2) from the rest]

1. **a.** Write the structure of 4-chloro-2-methylbenzaldehyde and mention how many signals will be obtained in the **DEPT-45&DEPT-90** spectra of the molecule. **5**

   b. In the mass spectrum of a Cl-containing compounds, two molecular ion peaks (M^+ and M^++2) appear. What is the approximate intensity ratio of these peaks? [natural abundance of ^{35}Cl and ^{37}Cl isotopes, approximately 75% and 25%, respectively]. **3+2=5**

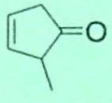
2. **a.** Depict the probable ^{13}C NMR (proton-decoupled) spectra of ethyl acetate and methyl propionate. **4+6=10**

   b. How many peaks the following molecule will show in proton-decoupled ^{13}C NMR spectrum? Depict the COSY spectrum of butan-2-one.

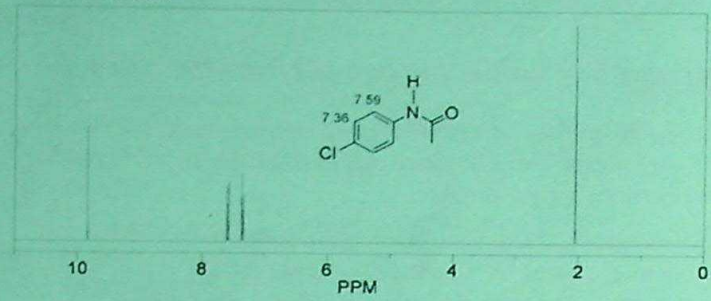
3. a. Draw the proton-decoupled ^{13}C-NMR spectra of the following compound **4+3+3 =10**

   CH_2FCHF_2 [Given: $^1J_{(C\text{-}F)}$ = 180 Hz, $^2J_{(C\text{-}F)}$ = 40 Hz; δ (50 MHz, $CDCl_3$, ppm): 90, 122].

   b. If the $^1J_{C\text{-}H}$ = 160 Hz, how many signals will be there in the **INEPT 80 & INEPT 120** spectra of the following molecule?



c. Draw the NOESY spectrum of the compound given here with its ^1H NMR



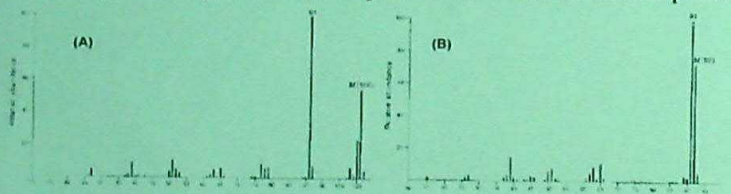
4. a. Draw the EI-MS and CI-MS spectra of 3,4-Dimethoxyacetophenone and compare them. **4+4+2 =10**

b. What is MALDI in mass spectrometry? Describe its significant points.

c. Describe TOF analyzer.

5. a. Draw the expected mass spectra for cumene and n-propylbenzene.Identify and compare the molecular ion peaks and base peaks for both compounds.Determine which one of the two compounds is likely to undergo McLafferty rearrangement, and explain the mechanism behind this fragmentation process. **4+4+2 =10**

b. In the provided mass spectra for ortho-xylene and toluene, assign each spectrum to its corresponding compound and, specify the fragment ion responsiblefor each labelled peak.



c. In the EI mass spectrum of isooctane, at which m/z value does the base peak appear, and which fragment ion is responsible for this peak?

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