# 2023

## M.Sc.

## 4th Semester Examination

### CHEMISTRY

### PAPER : CEM-401

### ( Spectroscopy )

*Full Marks* : 40

*Time* : 2 hours

*The figures in the right-hand margin indicate marks.*

*Candidates are required to give their answers in their own words as far as practicable.*

*Illustrate the answers wherever necessary.*

Answer from **all** the Groups as directed.

### GROUP—A

**1.** Answer *any* **four** questions from the following : 2×4=8

*(a)* What is the full form of DEPT? How is it useful?

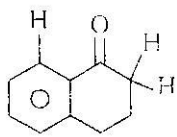
(b) Compound B shows only one $^1$H-NMR peak at $d$ = 2·2 (18H, s). Suggest a probable structure.

(c) How can you characterize *A*, *B*, *P* and *Z* form of DNA by circular dichroism spectroscopy?

(d) Establish the relation $E_R = \frac{E^2}{2M_0C^2}$, where the symbols have their usual meanings.

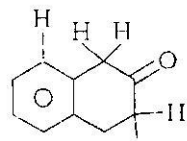
(e) How does spin-lattice relaxation affect the NMR peaks?

(f) How will you distinguish between **I** and **II** by $^1$H NMR?



**I**

and



**II**

## GROUP—B

**2.** Answer *any* **four** questions from the following : 4×4=16

(a) An organic compound having molecular formula $C_9H_8O_2$ shows following spectral data $^1$H NMR-δ(12·7, 1H, brs); δ(7·8, 1H, d, J = 18 Hz), δ(7·56, 5H, m); δ(6·45, 1H, d, J = 18 Hz), IR-1680 $cm^{-1}$, 2520-3070 $cm^{-1}$ (broad). Draw the structure of the compound.



( Continued )

(b) How will the NMR spectrum of an organic sample recorded in a 400 MHz NMR spectrometer differ from the NMR spectrum recorded in a 100 MHz NMR spectrometer?

(c) For the compounds $K_4[Fe(CN)_6]$ and $K_3[Fe(CN)_6]$, two types of Mössbauer spectra are observed. One spectrum shows a doublet whereas the other shows a singlet. Assign these spectra to the respective compounds.

(d) What is the McLafferty rearrangement in the mass spectral fragmentation of organic compounds? Give examples. Using appropriate deuterium labeled compound, prove that in McLafferty rearrangement always $\gamma$-hydrogen transfers.

(e) An organic compound having molecular formula $C_5H_8O$ shows following spectral data $^1H$ NMR $\delta$ : (6·2, 1H, d, $J$ = 17 Hz); $\delta$ (5·4, 1H, m, $J$ = 17 Hz); $\delta$ (2·3, 3H, s); $\delta$ (1·9, 3H, d), IR-1685 $cm^{-1}$, 3020 $cm^{-1}$, UV-VIS-$\lambda_{max}$(EtOH) = 277 nm, $\varepsilon_{max}$ = 4600. Draw the structure of the compound.

(f) What is NMR shift-reagent? Give an example and explain the mechanism of its activity.

## GROUP—C

**3.** Answer *any* **two** questions from the following : 8×2=16

(a) Compound **P** ($C_8H_{12}O_4$) shows the following $^1H$ NMR spectral data : $^1H$ NMR (δ) : 6·80 (s, 2H), 4·25 (q, $J$ = 7 Hz, 4H), 1·30 (t, $J$ = 7 Hz, 6H). Suggest a possible structure with explanation. 8

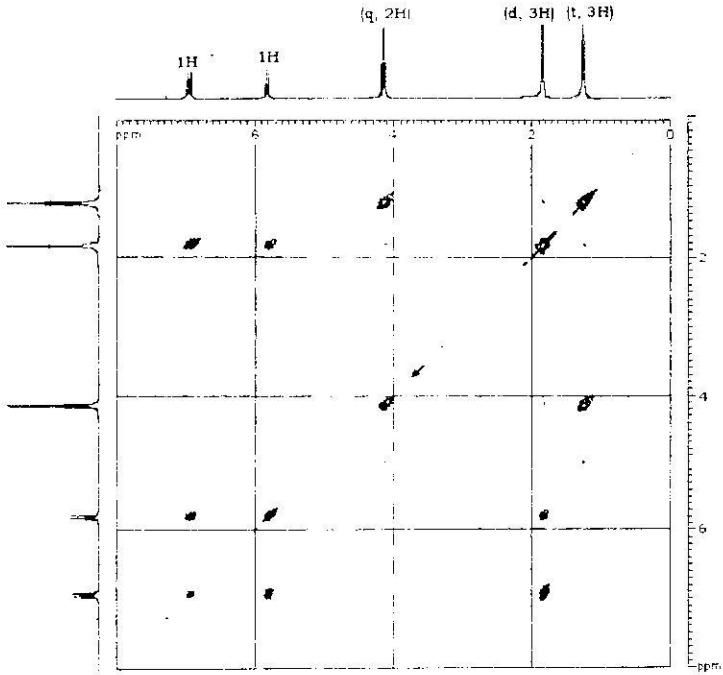
(b) (i) An organic compound having molecular formula $C_4H_6O_2$ shows a very strong IR band at 1720 $cm^{-1}$ and only one singlet signal in its $^1H$ nmr spectra. Draw the structure of the compound.

(ii) An organic compound having molecular formula $C_{10}H_{12}O_2$ shows following spectral data $^1H$ nmr-δ (8·0, 2H, m); δ (7·2, 3H, m); δ (5·2, 1H, m); δ (1·3, 6H, d), IR- 1730 $cm^{-1}$, 3050 $cm^{-1}$ and 2950 $cm^{-1}$. Draw the structure of the compound. 4+4=8

(c) (i) Write short notes on different types of polarized light.

(ii) What are the characteristics CD band observed for the identification of alpha helix, beta sheet and Random coil? 4+4=8

*(d)* A compound having molecular formula $C_6H_{10}O_2$ shows the following 2D COSY NMR spectrum. Assign the structure. 8

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