2022

M.Sc.

4th Semester Examination (CCAE) CHEMISTRY

PAPER—CEM-401

ADVANCED SPECTROSCOPY-II

Full Marks: 40

Time: 2 Hours

The figures in the margin indicate full marks.

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

Illustrate the answers wherever necessary.

Group-A

Answer any four questions.

4×2

- 1. Write note on NMR relaxation times.
- Explain why NMR sensitivity is increased when the applied magnetic field is increased.
- 3. What is meant by anisotropic effect? Draw a diagram for the anisotropic effect of ethylene.

(Turn Over)

- 4. Write down the name of software for the analysis of secondary and tertiary protein structure.
- 5. What is the unit of molar ellipticity?
- **6.** Explain how salicylic acid and its *meta* isomer can be distinguished by mass spectrometric analysis.

Group-B

Answer any four questions.

4×4

- 7. Illustrate 'double irradiation' with a suitable example.
- 8. Draw the diagram of an EI mass spectrometer.
- **9.** Explain how 2-butanone and butyraldehyde can be differentiated by mass spectrometry.
- 10. The ¹H NMR spectrum of a solution of 1,3-dimethylcyclopentadiene in conc. sulphuric acid shows three signals with relative intensities of 6:4:1. Propose an explanation for the appearance of the spectrum.
- 11. Write short notes on different types of polarized light.
- 12. Write down the criteria for the preparation of sample for CD spectroscopy.

Group-C

Answer any two questions.

 2×8

13. Propose a structure for the product A of the following reaction from the given data.

$$OH \longrightarrow C_7H_{12}O (A)$$

The spectral data for product [A]: IR: 1729 cm^{-1} ; 1H NMR (δ): ¹H NMR: 9.72 (d, 1H), 2.30 (sex, 1H), 1.4-18 (m, 10H). Note that the signals for 10H overlapping are due to both equivalent and non-equivalent hydrogens.

14. Assign a δ value to each of the indicated hydrogens of the following structures.

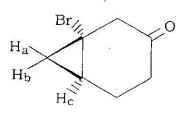
The possible numbers are 4.3, 6.3, 7.00, 7.32, 7.4, 7.65. Justify your assignments.

$$H$$
 CO_2Me O H

C/22/MSc/CCAE/4th Sem/CEM-401

(Turn Over)

15. For the compound below.



$$J_{ab} = 5.3 Hz$$
 $J_{ac} = 8.3 Hz$ $J_{bc} = 10.7 Hz$

- (i) how many ¹H NMR signals would you expect for the molecule?
- (ii) H_a appears as a dd at 1.32 ppm. Draw a labelled splitting tree diagram for H_a using the given coupling constant values.
- (a) Explain Nuclear Zeeman Effect in Mössbauer spectroscopy.
 - (b) Differentiate between $K_4[Fe(CN)_6]$ and $Na_2[Fe(CN)_5NO]$ by Mössbauer spectroscopy.

4+4