

(For candidates admitted from 2016–2017 onwards)

M.Sc. DEGREE EXAMINATION, NOVEMBER 2022.

Chemistry

## PHYSICAL METHODS IN CHEMISTRY – I

Time : Three hours

Maximum : 75 marks

## SECTION A — (10 × 2 = 20)

Answer ALL the questions.

1. What are stoke's and antistoke's lines?
2. State mutual exclusion rule.
3. What are fluxional molecules?
4. Name the factors that affect the NMR chemical shift.
5. What is positional isomerisation?
6. What is bathochromic shift?
7. How many ESR lines will appear for naphthyl naidcal?

17. What is double resonance technique? Explain how it is helpful in simplifying the NMR spectra.

18. A compound with molecular formula,  $C_9H_{11}O_2N$  shows the following spectral data. Determine the structure.

Mass : m/z 165, 137, 120, 92

$^1HNR$  : S 7.9 (d,  $J=8Hz$ , 2H), 6.6 (d,  $J=8Hz$ , 2H), 4.3 (q,  $J=6Hz$ , 2H) 4.0 (br, s, 2H,  $D_2O$ , exchangeable) 1.4 (t,  $J=6Hz$ , 3H).

19. Explain Mc Lafferty rearrangement and discuss the fragmentation pattern of ketones and aldehydes.

20. Write notes on : (a) Combridge structural Database (CSD) and (b) Protein Data Bank (PDB)

8. What is positive cotton effect?
9. What is atomic density and electron density?
10. How will you determine the sharpness of lines in powder diffractometer?

SECTION B — ( $5 \times 5 = 25$ )

Answer ALL questions, choosing either (a) or (b)

11. (a) Explain the effect of isotopic substitution on the rotational spectrum of a diatomic molecule.

Or

- (b) Write short notes on: (i) Fortrat diagram (ii) Parallel and perpendicular vibrations.
12. (a) How will you account for the observed spin-spin splitting and chemical shift in the NMR spectrum of an AX system?

Or

- (b) Write short note on NOE in NMR and give its importance.

13. (a) How will you differentiate primary, secondary and tertiary amines using IR spectroscopy?

Or

- (b) Discuss the UV-visible spectral features of disubstituted benzene molecule.
14. (a) Write note on FAB method of mass spectrometry.

Or

- (b) Discuss the applications of CD in determining the absolute configuration of optically active compound.
15. (a) Explain the following: (i) Glide planes (ii) Screw axes (iii) Structure factor.

Or

- (b) How will you elucidate the structure by neutron diffraction?

SECTION C — ( $3 \times 10 = 30$ )

Answer any THREE questions.

16. (a) Write the selection rules for harmonic and anharmonic oscillators.
- (b) Explain the terms overtones, hot bands and combination bands and give the corresponding expressions for it.