

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, December 2025

**Chemistry / Analytical Chemistry / Polymer Chemistry / Chemistry with
Specialisation in Drug Design and Development**

CH 233/CL 233/PC 233/CHDD 533 – PHYSICAL CHEMISTRY – III

(2020 Admission Onwards)

Time : 3 Hours

Max. Marks : 75

SECTION – A

Answer **any two** sub-questions among (a), (b), or (c) from each question.

Each sub-question carries **2** marks.

1. (a) Why approximate methods are used in quantum mechanical treatment?
(b) What is the secular equation?
(c) What is meant by Fock matrix?
2. (a) What is the Chapman equation?
(b) Discuss the translational degree of freedom of gas.
(c) What is the short range order of structures?
3. (a) How is the Fourier transform used in spectroscopy?
(b) What is the selection rule for ESR spectroscopy?
(c) What is the principle of NQR spectroscopy?
4. (a) What is the principle of minimum entropy production?
(b) What is the effect of temperature on the ternary phase diagram?
(c) What is meant by electro-osmosis?
5. (a) What are Gaussian type orbitals?
(b) What is Roothan concept?
(c) What is the RHF method?

(10 × 2 = 20 Marks)

P.T.O.

SECTION – B

Answer either (a) or (b) of each question.

Each question carries **5** marks.

6. (a) Discuss the variation theorem and its proof.
(b) Explain the Born-Oppenheimer approximation and its limitations.
7. (a) What are the various inter molecular forces of gases?
(b) Describe the barometric method of measuring vapour pressure.
8. (a) Discuss the analytical applications of ESR spectroscopy.
(b) Describe the instrumentation of Fourier transformation NMR Spectroscopy.
9. (a) Explain the general theory of non-equilibrium processes.
(b) Discuss the application of irreversible thermodynamics to diffusion.
10. (a) Discuss the Huckels methods in computation chemistry.
(b) Discuss the “Arguslab” software and its advantages.

(5 × 5 = 25 Marks)

SECTION – C

Answer **any three** questions. Each question carries **10** marks

11. Compare Molecular Orbital and Valance Bond theories.
12. (a) Illustrate the vacancy model for a liquid.
(b) Discuss the determination of surface tension of a liquid by drop weight method.
13. Explain the principle, working and uses of X-ray photoelectron spectroscopy
14. Explain the phase diagram of three component liquid systems with one pair of partially miscible liquids
15. (a) Construct Z-matrix for H₂O molecule.
(b). Explain the Density functional theory method.

(3 × 10 = 30 Marks)