

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, March 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 question carries **2** marks.

1. (a) What is the Hartree-Fock field theory?
(b) What does the Born-Oppenheimer approximation do?
(c) Discuss quantum mechanical treatment of hybridization
2. (a) What is the relationship between the temperature and the molecules velocity?
(b) What is the significance of the Virial equation?
(c) Discuss the vibrational degree of freedom of gaseous molecules.
3. (a) What is the role of Fourier transform in NMR spectroscopy?
(b) What is Kramer's rule?
(c) What is the magnetic interaction in Mössbauer spectroscopy?

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4. (a) What is Onsager reciprocal equation?
(b) What is the Prigogine effect?
(c) What is entropy production due to matter flow?
5. (a) What are Gaussian - type orbitals?
(b) Describe the Restricted open-shell Hartree-Fock method.
(c) What are the advantages of CHARMM force field?

(10 × 2 = 20 Marks)

SECTION – B

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

Each question carries 5 marks.

6. (a) Explain the concept of variation theorem.
(b) What is Valence Bond Theory? How is it differing from Molecular Orbital Theory?
7. (a) Discuss the dynamic methods of measuring vapour pressure of a liquid.
(b) Describe the drop number method for the determination of surface tension of a liquid.
8. (a) Describe the experimental aspects of NMR spectroscopy.
(b) What is ENDOR? How is it differing from ELDOR?
9. (a) What is thermo-osmosis? What is its application?
(b) Discuss the influence of temperature on three component systems
10. (a) What are diffuse basis sets? How are they differing from polarized basis sets?
(b) Discuss the importance and applications of Density Functional Theory.

(5 × 5 = 25 Marks)



SECTION – C

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

11. (a) Explain the molecular orbital diagram of Be_2 .
(b) Describe the application of HMO method to butadiene,
12. Explain the various types of degrees of freedom of gaseous molecules
13. (a) Explain the principle and applications of Mossbauer spectroscopy
(b) What is the X-ray photoelectron spectroscopy? What are its applications?.
14. (a) What are electro-kinetic effects? What is its application?
(b) Sketch the graphical representation of three component system.
15. Explain the Quantum mechanical computational methods used in chemistry.

(3 × 10 = 30 Marks)

