Reg. No. : .....

Name : .....

## Third Semester M.Sc. Degree Examination, February 2024 Chemistry/Analytical Chemistry/Polymer Chemistry CH 233/CL 233/PC 233 : 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) What is a secular equation?
  - (b) What is the principle of the Hartree-Fock method?
  - (c) Describe the VB treatment of Hydrogen molecule.
- 2. (a) What is the derivation of Maxwell velocity distribution function?
  - (b) Discuss the various factors that the degree of freedom of gas molecules depend.
  - (c) Discuss the vacancy model of a liquid.
- 3. (a) Discuss the population of energy levels in proton NMR.
  - (b) What are the advantages of applying Fourier Transformation in NMR studies?
  - (c) Discuss the principle and applications of Mossbauer spectroscopy.

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- 4. (a) What is the principle of minimum entropy production?
  - (b) What is the significance of irreversible thermodynamics?
  - (c) What is mean by electro-kinetic effect?
- 5. (a) What is Roothaan concept in computational chemistry?
  - (b) What is a minimal basis set?
  - (c) What is CHARMM used for?

 $(10 \times 2 = 20 \text{ Marks})$ 

## 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) What is the concept of MO theory? Point out the difference between Valance Band and Molecular Orbital Theories.
- 7. (a) Briefly explain the various inter molecular forces acting in gases.
  - (b) Discuss the barometric method of measurement of vapour pressure.
- 8. (a) What is the principle of ESR spectroscopy? What are its analytical applications?
  - (b) What is ENDOR spectroscopy? How is it differing from ELDOR spectroscopy?
- 9. (a) Discuss the various methods of entropy productions.
  - (b) Describe the phase diagram of two salts and water system with double salt formation.
- 10. (a) What are Slater type orbitals? How can they be distinguished from Gaussian type orbitals?
  - (b) Illustrate the Density functional theory method.

(5 × 5 = 25 Marks)

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## SECTION - C

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

- 11. (a) Explain the Bon-Oppenheimer approximation.
  - (b) Describe the Hückel molecular orbital theory for ethylene.
- 12. Explain the various methods for the determination of surface tension of a liquid.
- 13. Explain the instrumentation and experimental aspects of NMR spectroscopy.
- 14. Explain the applications of irreversible thermodynamics.
- 15. Explain the various Quantum mechanical computational methods.

(3 × 10 = 30 Marks)