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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 × 2 = 20 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)

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.

($3 \times 10 = 30$ Marks)

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