(Pages : 3) H - 4111

| Reg. No. | : | ••••• | |
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Third Semester M.Sc. Degree Examination, January 2020 Chemistry/Polymer Chemistry

CH/CL/CM/CA/PC 233: PHYSICAL CHEMISTRY - III

(Common for Chemistry (2016 Admission Onwards) and Polymer Chemistry (2018 Admission)

Time: 3 Hours Max. Marks: 75

PART – A

Answer **any two** among **A**, **B** and **C** of each question. Each sub question carries **2** marks.

- 1. (A) State variation theorem.
 - (B) Draw the MO diagram of HF.
 - (C) Calculate the bond order of O₂, F₂ and CO.
- 2. (A) Explain the terms in $6 31 + G^*$.
 - (B) Differentiate between RHF, ROHF and URHF.
 - (C) Write any two drawbacks of MM method.
- 3. (A) Define nuclear resonance.
 - (B) What are the requirements of Mossbauer spectroscopic analysis?
 - (C) State the principle of NQR spectroscopy.

- 4. (A) What are the limitations of Einstein's theory of heat capacity of solids?
 - (B) Explain Dulong and Petit's law.
 - (C) Explain the significance of principle of equipartition of energy.
- 5. (A) Explain Calomel electrode.
 - (B) What is the principle behind coulometry?
 - (C) What are the applications of AAS?

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

PART - B

Answer either **A** or **B** of each question. Each question carries **5** marks.

- 6. (A) Apply variation theorem for particle in ID box and calculate the ground state energy.
 - (B) Apply HMO method to benzene and explain the bonding.
- 7. (A) Write the Z-matrix of CH₃CHO and NH₃.
 - (B) Explain Hohenberg-Kohn theorem of DFT calculations.
- 8. (A) Explain briefly the instrumentation of NMR spectroscopy.
 - (B) Explain Kramer's degeneracy.
- 9. (A) Derive statistically the relation between probability and entropy.
 - (B) Derive the expressions for molecular partition functions.
- 10. (A) How can you find the pH of a solution by using glass electrode?
 - (B) Explain the principle of polarography.

 $(5 \times 5 = 25 \text{ Marks})$

PART - C

Answer any three questions. Each question carries 10 marks.

- 11. Explain quantum mechanical treatment of sp³ hybridization for alkanes.
- 12. What are basis sets and explain different types of basis sets.
- 13. How can you differentiate (i) low spin and high spin complexes and (ii) oxy and deoxy hemoglobin by Mossbauer spectroscopy?
- 14. Express the thermodynamic properties in terms of partition functions.
- 15. How can you estimate the mass of copper from copper sulphate solution by using electrogravimetry?

 $(3 \times 10 = 30 \text{ Marks})$