

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, March 2022

Chemistry/Polymer Chemistry/Analytical Chemistry

CH/CL/PC 233 : PHYSICAL CHEMISTRY – III

(2020 Admission)

Time : 3 Hours

Max. Marks : 75

SECTION – A

Answer **two** among (a), (b) and (c) from each. Each sub question carries **2** marks.

- State and explain variation theorem.
 - Find the spectroscopic term symbols for Li_2 and O_2 .
 - Define Fock operator. What is its significance?
- Estimate C_v of HCl and CO_2 in $\text{JK}^{-1} \text{mol}^{-1}$ by applying equipartition principle.
 - State the physical significance of van der Waals constants and give their units.
 - Define mean free path. Calculate the mean free path of oxygen gas in nm at 25°C and 1 atm pressure if the collision diameter is 360 picometer.
- Draw the NQR energy levels with energies, if the nuclear spin value is $3/2$. Explain the impact of quadrupole interactions on NMR lines.
 - What are the information that can be gained from photoelectron spectroscopy?
 - What is FID? What are the advantages of FTNMR?

P.T.O.



4. (a) Write a note on phenomenological relations in irreversible thermodynamics.
(b) Write a note on Onsagar reciprocal relations.
(c) What is mean by thermoelectric phenomena?
5. (a) Compare 6-31G++ and 6-31++ G.
(b) How is force field different from basis set?
(c) What is a stationary point? Mention its relevance.

(10 × 2 = 20 Marks)

SECTION – B

Answer either (a) or (b) from each question. Each sub question carries **5** marks.

6. (a) Discuss the quantum mechanics of sp hybridization with an example.
(b) Apply Huckel's molecular orbital theory to ethylene.
7. (a) Define surface tension and viscosity and methods used to determine them.
(b) Derive expressions for average velocity and root mean square velocity.
8. (a) Explain Larmor precession and its importance in resonance techniques. A system of protons at 25°C is placed in a 2T magnetic field. Find the ratio of protons in upper to lower state if nuclear g factor value is 5.585 and nuclear magneton is $5 \times 10^{-27} \text{ JT}^{-1}$.
(b) Give the applications of ESR spectroscopy in studying reaction rates and mechanism and for analytical purposes.
9. (a) What is mean by thermoelectric phenomena?
(b) Write a note on Glansdorf- Pregogine equation and its significance.
10. (a) Explain in detail various post HF methods used in computational studies.
(b) Write a note on any three force fields highlighting their applications

(5 × 5 = 25 Marks)



SECTION – C

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

11. Apply valence bond theory to hydrogen molecule.
12. Write an essay on the transport properties and intermolecular forces of gases.
13. Explain the basic principles and applications of Mossbauer spectroscopy. Give the quadrupole and magnetic hyperfine interactions.
14. Sketch and explain the graphical representation of a three-component liquid-liquid system with
 - (a) one pair of partially miscible liquids;
 - (b) two pairs of partially miscible liquids;
 - (c) three pairs of partially miscible liquids.
15. (a) How is semi empirical method different from dft method? Explain in detail.
(b) Explain in detail the theory, design constrain and applications of MD simulations.

(3 × 10 = 30 Marks)

