January 2023

M.Sc. (Chemistry) Ist SEMESTER

Physical Chemistry (General–I) (CH-103B)

Time : 3 Hours]   [Max. Marks : 75

Instructions :

1. *It is compulsory to answer all the questions (1.5 marks each) of Part-A in short.*

2. *Answer any four questions from Part-B in detail.*

3. *Different sub-parts of a question are to be attempted adjacent to each other.*

4. *Use of non programmable scientific calculator is allowed.*

PART–A

1. (a) Derive expression for $\left(\dfrac{d}{dx}+x\right)^2$.   (1.5)

    (b) Write expression for thermodynamic probability for FD statistics.   (1.5)

    (c) What will happen if walls of one dimensional box are suddenly removed?   (1.5)

    (d) Write expectation values of x, x^2, P_x, P_x^2.   (1.5)

    (e) Distinguish reversible and irreversible processes in thermodynamics.   (1.5)

(f) Calculate minimum energy for an electron confined to a molecule of length 1 nm. (1.5)

(g) Write Schrödinger equation for 3D box. (1.5)

(h) What do you mean by eigen function and eigen values? (1.5)

(i) Discuss criteria for spontaneity of a process in brief. (1.5)

(j) Calculate the probability of finding the particle between 0.49a and 0.51a for Ψ_1 and Ψ_2. (1.5)

PART–B

2. (a) Solve Schrödinger wave equation for hydrogen-like particles. (10)

(b) Explain the concept of degeneracy in case of three dimensional box. (5)

3. (a) Explain quantum tunneling in details. (5)

(b) Discuss free energy functions and their significance in details. (10)

4. Find expressions for most probable distribution of N number of particles among various energy levels according to BE statistics. (15)

5. (a) Do a comparison for M-B, BE and FD statistics. (5)

(b) Discuss Schrödinger equation for a particle in a box and find expression for zero point energy, and normalized wave function and probability function. (10)

6. (a) Explain shapes of s, p and d-orbitals with the help of θ and Φ functions. (10)

(b) Calculate value of Lagrange's undetermined multipliers α and β. (5)

7. What do you mean by partial molar quantities? Drive expression for Chemical Potential, free energy, and volume. Also derive Gibb's-Duhem equation. (15)

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