UUCMS. No.

B.M.S. COLLEGE FOR WOMEN
BENGALURU – 560004

I SEMESTER END EXAMINATION-APRIL – 2024

M.Sc. CHEMISTRY-PHYSICAL CHEMISTRY-I
(CBCS Scheme-F+R)

Course Code: MCH103T   **QP Code: 11009**
Duration: 3 Hours   **Max. Marks: 70**

Instruction: Answer Question No.1 and any FIVE of the remaining.

1. Answer any *TEN* questions   **(2×10=20)**

a) Define the operators ∇ and ∇^2.

b) Show that Harmiltonian operator is Hermitian provided that the wave function is well behaved.

c) Give the solution for the Schrodinger wave equation for a particle in 3D box.

d) What is quantum mechanical tunneling?

e) Which of the following is the eigen function of the operator d^2/dx^2 (i) 6cos4x (ii) $5x^2$

f) Explain the term symbol with an example.

g) Calculate the steric factor for a reaction having the k = 3.22 x 10^{-2} s^{-1} with the Ea= 290 $kJmol^{-1}$ and the collision number 0.325 x10^{14} at 298 K.

h) Mention the limitation of the collision theory.

i) When water is subjected to temperature-jump method, the relaxation time to return to the equilibrium is 60µs. Calculate rate constants for the forward and reverse reaction.

j) Give BET adsorption equation and explain the terms involved in it.

k) Represent the Lineweaver-Burk plot and explain its significance.

l) Mention the differences between thermal and photochemical reactions.

2. a) Set up and solve Schrondinger equation for a rigid rotator.

b) Formulate the time- independent Schrondinger equation.   **(5+5=10)**

3. a) Give quantum mechanical interpretation of Pauli's exclusion principle.

  b) Apply variation method for a particle in a one-dimensional box.　　　　　**(5+5=10)**

4. a) Discuss the kinetics and mechanism of photochemical reaction of hydrogen and chlorine.

  b) Outline flash photolysis technique in the study of rapid reactions.　　　　　**(5+5=10)**

5. a) Discuss the Lindemann's theory of unimolecular reactions and mention its limitations.

  b) Derive Gibbs adsorption isotherm equation.　　　　　**(6+4=10)**

6. a) Apply perturbation theory to He like atom and find its solution.

  b) Deduce the rate expression for the influence of primary salt on the rate of reaction.

　　　　　(5+5=10)

7. a) Represent the total wave functions for the 1s, 2p and 3s orbitals of hydrogen atom.

  b) Obtain Laplace equation for pressure difference of curved surface.

  c) What are radial angular distribution functions? Mention their significance.　　　　　**(4+3+3=10)**

8. a) Write a note on mechanical adsorption.

  b) Write the Slater determinant wave function for the ground state of Li atom and show that

   the configuration $1s^3$ is not valid.

  c) Explain the effect of inhibitor on the enzyme catalyzed reaction.　　　　　**(4+3+3=10)**

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