November 2025
M.Sc.
First Semester
CORE – 03
CHEMISTRY
Course Code: MCHC 1.31
(Physical Chemistry - I)

Total Mark: 70 *Pass Mark: 28*
Time: 3 hours

Answer five *questions, taking* one *from each unit.*

UNIT–I

1. (a) Prove that a state function which is not an eigenfunction of a Hermitian operator $\hat{A}$ can be written as a linear combination of a set of eigenfunction. 3
   (b) Explain the uncertainty principle with the help of a neat diagram. 4
   (c) Solve the wave equation of hydrogen atom using Schrödinger equation. 7

2. (a) What is Lagrange's equation of motion? Explain. 3
   (b) Derive an expression for the energy of a rigid rotor. 6
   (c) Explain the energy eigenvalue equation. 3
   (d) What are eigenfunctions and eigenvalues? 2

UNIT–II

3. (a) State and prove the variation theorem. 5
   (b) What is Born-Oppenheimer approximation? 2
   (c) Construct the wave functions for the sp^3 hybrid orbitals. 5
   (d) Write the Huckel secular equation for 1,3-butadiene. 2

4. (a) Give the MO treatment of the hydrogen molecule. 5
   (b) Explain the Pauli antisymmetry principle. 6
   (c) Draw the HMO diagram of ethylene and give its secular equation. 3

UNIT–III

5. (a) What are surfactants? How are they classified? 4
   (b) Discuss and derive the BET equation for multilayer adsorption. 6
   (c) For a 1.0×10^{-4} M aqueous solution of n-butanoic acid, $d\gamma/dc = -0.080\ Nm^2\ mol^{-1}$ at 25°C. Using the Gibbs adsorption equation, determine the surface excess of butanoic acid and also calculate the average surface area available to each molecule. 4

6. (a) How does chemisorption differ from physisorption? Explain the factors which affect the adsorption of a gas on a solid. 4
   (b) Derive the expression of Gibbs adsorption isotherm for a liquid system. 6
   (c) What do you understand by hydrophobic interaction in a surfactant? Explain. 4

UNIT–IV

7. (a) What is axis of symmetry? Explain the various type of axes of symmetry in a crystal. 5
   (b) Derive the Bragg equation for diffracting X-rays by crystals. 5
   (c) Calculate the Miller indices of crystal planes which cut through the crystal axes at 4
      (i) (2a, 3b, c)
      (ii) (6a, 3b, 3c)

8. (a) What is superconductivity? Explain the different types of superconductivity. 6
   (b) Write a short note on each of the following: 2×2=4
      (i) Colour centres
      (ii) Subtractional solid solutions
   (c) Calculate the angle at which first order reflection and second order reflection will occur in an X-ray spectrometer when X-rays of wavelength 1.54 Å are diffracted by the atoms of a crystal having interplanar distance of 4.04 Å. 4
   (Given, $\sin^{-1}(0.191) = 10°\ 51'$, $\sin^{-1}(0.381) = 22°\ 24'$.)

UNIT–V

9. (a) Briefly explain the mechanism of absorption and emission of electromagnetic radiation. 3

   (b) Derive the expression for the rotational energy level taking diatomic molecules as a rigid rotator. 7

   (c) What is the moment of inertia of a diatomic molecule whose internuclear distance is 150 pm and the reduced mass is 1.5×10^{-27} kg? 4

10. (a) Taking diatomic molecule as a simple harmonic oscillator, show that the energy for the lowest vibrational level (E_0) is not equal to zero. 6

    (b) Discuss the different rotational spectra in the case of polyatomic molecules. 4

    (c) What do you understand by pure rotational Raman spectrum of diatomic molecules? Explain. 4