2023
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) What is a Hermitian operator? Prove that if the eigenfunction of a Hermitian operator has different eigenvalues, then they are orthogonal. 4
   (b) State and explain the third postulate of quantum mechanics. 3
   (c) Solve the wave equation of hydrogen atom using Schrödinger equation. 7

2. (a) Discuss the uncertainty principle. 4
   (b) What are orthogonal and normalised wave function? Write the properties of well-behaved wave function. 4
   (c) Derive an expression of a harmonic oscillator using quantum mechanics. 6

UNIT–II

3. (a) Discuss the valence bond treatment of H_2. 6
   (b) Explain in detail the anti-symmetry principle. 6
   (c) What is Born-Oppenheimer approximation? 2

4. (a) Give the application of variation method. 4
   (b) Construct the wavefunctions for the sp^2 hybrid orbitals. 3
   (c) Discuss the MO treatment of the hydrogen molecule. 5
   (d) Write the secular determinant for ethylene using Huckel MOT. 2

UNIT–III

5. (a) What are the factors that contribute to the strength of hydrophobic interaction? 4
   (b) Explain the process of wetting using Young-Dupre equation. 3
   (c) Give the derivation of BET equation. 7

6. (a) Explain the thermodynamic parameters of micellization. 4
   (b) Derive an expression for Gibbs adsorption isotherm. 5
   (c) What is Kelvin equation? Explain. 2
   (d) What are surfactants? Give their classification. 3

UNIT–IV

7. (a) Find the Miller indices of 4
      (i) the sets of planes intersecting the axes represented by labels $\left(\frac{4}{3}, \frac{3}{2}, \infty\right)$ and $(-2, 1, \infty)$.
      (ii) The planes that intersects the crystallographic axes at the distance $(6a, 4b, 2c)$ and $(3a, \infty b, \infty c)$.
   (b) Discuss the Kroger-Vink notation for crystal defects. Give examples. 6
   (c) Write a note on p-n junction. 4

8. (a) What are colour centres? How do they arise? 4
   (b) With the help of a neat diagram explain the extrinsic semiconductors. 4
   (c) What are the different types of defects? Explain point defect in detail. 5
   (d) Define the Bragg's law. 1

UNIT–V

9. (a) The rotational spectrum of HCl molecules shows that the rotational lines are equally separated by 20.70 cm^{-1}. Calculate the internuclear bond length. 4

(b) Write Morse equation for the energy of the vibrational levels of the anharmonic oscillator. Compare the potential energy curves of the anharmonic oscillator with the harmonic oscillator. 5

(c) Discuss the vibrational spectra of diatomic molecules. 5

10. (a) Which factors governs the intensities of rotational spectral in a rigid diatomic rotator? Illustrate using appropriate curves. 6

(b) What are Stokes and anti-Stokes lines? Explain. 3

(c) Write a note on interaction of light with matter. 3

(d) What is selection rule? Give the selection rule for pure rotational spectra. 2
