2021
M.Sc.
First Semester
CHEMISTRY
Course Code: MCHC 1.31
(Physical Chemistry - I)

Total Mark: 70   Pass Mark: 28
Time: 3 hours
Answer <u>five</u> *questions taking* <u>one</u> *from each Unit.*

UNIT–I

1. (a) Prove that if there exists a set of functions which are eigen functions of two operators $\hat{A}$ and $\hat{B}$ they must commute.   3

    (b) Discuss the uncertainty principle.   4

    (c) Solve the equation of hydrogen atom using Schrodinger equation.   7

2. (a) State and explain the third postulate of quantum mechanics.   2½

    (b) What is Hermitian operator? Examine if $\dfrac{d^2}{dx^2}$ is a Hermitian or not.   3

    (c) What is a normalized wave function? Write the properties of well-behaved wave function.   2½

    (d) Solve the equation for the harmonic oscillator quantum mechanically.   6

UNIT–II

3. (a) Write the molecular orbital theory for hydrogen molecule.   6

    (b) Solve the non-linear variation function equation.   5

    (c) Explain the correlation diagram of homonuclear diatomic molecules.   3

4. (a) Discuss Born-Oppenheimer approximation.   5

    (b) What are the approximations introduced in the Huckel theory?   6

    (c) What are symmetric and anti-symmetric wave functions? Explain. 3

UNIT–III

5. (a) Derive the BET equation.   7
   (b) Explain the Young-Dupre equation.   2
   (c) What are the factors that contribute to the strength of hydrophobic interaction?   4
   (d) Define surface free energy.   1
6. (a) Derive the Gibbs adsorption isotherm equation.   5
   (b) What is micellization? Explain the thermodynamic parameters for its formation.   5
   (c) What is capillary action? If water at 25ºC rises through 7.36 *cm* in a capillary of radius 0.2 *mm*, what is its surface tension at that temperature? ($p = 997.1 \text{ kg m}^{-3}$)   2+2=4

UNIT–IV

7. (a) What are the different types of defects? Discuss point defect in detail.   5
   (b) Find the Miller indices of
      (i) the sets of planes intersecting the axes represented by labels
      $$\left(\frac{1}{2}, \frac{1}{3}, \infty\right) \text{ and } (-1, 1, \infty)$$
      (ii) the planes that intersects the crystallographic axes at the
      distance $(3a, 2b, c)$ and $(2a, \infty b, \infty c)$ 4
   (c) What are extrinsic semi conductors? Discuss briefly giving diagrams.   3
   (d) Diffraction angle θ equal to 8.4° for a crystal having interplanar distance in the crystal is 0.400 *nm* when first order diffraction was observed. Calculate the wavelength of X-ray used. (Given 1 *nm* = 10^{-9} *m*)   2
8. (a) Discuss the Kroger-Vink notation for crystal defects. Give examples.   6
   (b) What are colour centres? How do they arise?   4
   (c) Write a note on p-n junction.   4

UNIT–V

9. (a) Which factors govern the intensities of rotational spectral lines in a rigid diatomic rotator? Illustrate using the appropriate curve.　　6

(b) Explain the vibrational spectra of diatomic molecules.　　5

(c) What are Stokes and anti-Stokes lines? Is the intensity of Stokes lines different from that of anti-Stokes lines? Explain.　　3

10. (a) What do you mean by selection rule? What is the selection rule for pure rotational spectra?　　2

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

(c) 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

(d) Which of the following molecules will show a pure rotational spectrum?

HCl, CO, CH_3Cl, H_2, NH_3, H_2O.　　3

———————————