Total number of printed pages = 8

63/1(SEM-5) CC12/CHMHC5126

2024

CHEMISTRY

Paper : CHMHC5126

(Physical Chemistry-V)

Full Marks : 60

Pass Marks : 24

Time : 3 hours

The figures in the margin indicate full marks for the questions.

1. Choose the correct answer: ***(any five)*** 1×5=5

   (a) Which of the following is IR-inactive but Raman active?

   (i) N_2

   (ii) SO_2

   (iii) HCL

   (iv) Protein

Contd.

(b) ESR spectrum is observed in

(i) Radio frequency region

(ii) IR-region

(iii) Microwave region

(iv) UV region

(c) The shift of an absorption maximum towards longer wave length is known as

(i) Hyperchromic shift

(ii) Hypochromic shift

(iii) Bathochromic shift

(iv) Hypsochromic shift

(d) Which of the following process is the reverse of a photochemical reaction?

(i) Chemiluminescence

(ii) Fluorescence

(iii) Phosphorescence

(iv) Photosensitization

(e) What will be the quantum yield when one mole of substance reacts by absorbing 6.023×10^{23} photons

(i) 0.1

(ii) 1

(iii) 10

(iv) 0

(f) The expression for Hamiltonian operator $\hat{H}$ is

(i) $h^2/8\pi^2 m\nabla^2 + V$

(ii) $\frac{-h^2}{8\pi^2 m}\nabla^2 + V$

(iii) $\frac{h^2}{8\pi^2 m}\nabla^2 - V$

(iv) $\frac{-h^2}{8\pi^2 m}\nabla^2 - V$

(g) The wave function for SP hybrid orbital is

(i) $\psi = \frac{1}{\sqrt{2}}(2S + 2P_x)$

(ii) $\psi = \frac{1}{\sqrt{3}}2S + \sqrt{\frac{2}{3}}\,2P_x$

(iii) $\psi = \frac{1}{\sqrt{2}}(2S - 2P_x)$

(iv) $\psi = \frac{1}{\sqrt{2}}2S + \frac{1}{\sqrt{3}}2P_x$

(h) Spin multiplicity can be calculated by using equation

(i) 2S-1

(ii) 2S+1

(iii) S+1

(iv) S-1

(i) The eigenvalue of the function $\psi = 8l^{4x}$ is

(i) l^{4x}

(ii) 32

(iii) 8

(iv) 4

(j) Splitting of spectral lines due to magnetic field is called

(i) Zeeman effect

(ii) Electromagnetic effect

(iii) Condensation effect

(iv) Spark effect

2. Answer the following questions : ***(any five)*** 2×5=10

(a) Show that $\sin 3x$ is not an eigen function of d/dx but it is an eigen function of d^2/dx^2. What will be the eigenvalue?

(b) Show that if two operators $\hat{A}$ and $\hat{B}$ are Hermitian, then their product $(\hat{A}\hat{B})$ is also Hermitian if and only if $\hat{A}$ and $\hat{B}$ commute.

(c) Write the Schrödinger equation in terms of Polar Co-ordinates.

(d) What are quantum numbers? Write the different types of quantum numbers.

(e) Write the difference between internal conversion and intersystem crossing.

(f) Calculate the normal modes of vibration of CH_4 and Co_2 molecule.

(g) What is chemiluminescence?

3. Answer *any five* the following questions : 5×5=25

(a) State and explain Lambert-Beer law for light absorption by solutions. Write its limitations. 1+3+1=5

(b) (i) Write a note on Larmor Precession. 2

(ii) What are magnetically equivalent and nonequivalent protons? 2

(iii) What do you mean by chemical shift in NMR-spectroscopy? 1

(c) (i) What are Stoke's and anti-Stoke's lines? 2

(ii) Write the selection rule for pure ratational Raman Spectrum of a diatomic molecule. 1

(iii) Write the advantages of Raman-spectroscopy over IR-Spectroscopy. 2

(d) Draw & discuss ESR spectrum of H-atom and CH_3 radical.

(e) Write the various elctronic transitions in electronic spectroscopy. Predict the kind of electronic transitions in CH_3Cl, Cl_2 and $\rangle C{=}O$ group. 2+3=5

(f) Derive the expression for the energy of a particle in a two-dimensional box. 5

(g) Discuss the valence bond theory of H_2.

(h) Write the postulates of quantum mechanics.

(i) (i) Normalize the function $\psi = x^2$ over the interval $0 \le x \le k$ (k is a constant) 3

(ii) Show that $\psi_1 = x$ and $\psi_2 = x^2$ are orthogonal over the interval $-k \le x \le k$ (k is a constant) 2

4. Answer ***any two*** of the following question: 10×2=20

(a) (i) Write the molecular electronic configuration of N_2 molecule and draw its energy level diagram also find its bond order. 1+2+1=4

(ii) What are binding and antibonding orbitals? Write the criteria of forming molecular orbitals from atomic orbitals. 2+2=4

(iii) Write the limitations of Valence bond theory. 2

(b) (i) Define quantum yield. Write two reasons of low and high quantum yield each. Give one example of photochemical reaction with extremly high quantum yield. 1+4+1=6

(ii) What three differences between fluorescence and phosphorescence with example. 3

(iii) What are photosensitized reaction? 1

(c) Write notes on : 3+2+3+2=10

(i) Nuclear spin-spin interaction

(ii) Auxochrome and Chromophore.

(iii) Principles of NMR spectroscopy.

(iv) Franck-Condon Principle.

(d) (i) Draw the radial probability distribution curves for 3S and 3P orbitals. 2

(ii) Write the differences between orbit and orbital. 2

(iii) Set up the Schrödinger wave equation for a simple harmonic Oscillator and solve it for the energy ligen values. 6