2026

(FYUGP)

(6th Semester)

CHEMISTRY

(MINOR)

Paper : CHEM M–6(T)

(Physical Chemistry—V : Quantum Chemistry and Spectroscopy)

Full Marks : 75

Pass Marks : 40%

Time : 3 hours

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

(PART : A—OBJECTIVE)

(*Marks* : 25)

SECTION—I

(*Marks* : 10)

Choose the correct option : 1×10=10

1. The rotational transitions for a rigid diatomic molecule are governed by the selection rule

(a) $\Delta J = \pm 1$

(b) $\Delta J = 1$

(c) $\Delta J \geq \pm 1$

(d) $\Delta J \leq \pm 1$

2. The molecular spectra arise from which of the following types of transition?

   (a) Electronic, rotational, vibrational and translational transitions

   (b) Rotational, vibrational and electronic transitions

   (c) Rotational, vibrational and translational transitions

   (d) None of the above

3. The statement 'one molecule is activated by the absorption of one quantum of radiation in the primary step of a photochemical reaction' is

   (a) Grotthuss-Draper law

   (b) Beer's law

   (c) Stark-Einstein law

   (d) Lambert's law

4. The instantaneous re-emitting of light from a substance when exposed to light and stops when the light is cut off is called

   (a) chemiluminescence

   (b) fluorescence

   (c) phosphorescence

   (d) photosensitization

5. Vibrational transitions exist in

   (a) microwave

   (b) visible region

   (c) infrared region

   (d) radiowave region of the spectrum

6. Raman effect arises due to

   (a) absorption of light

   (b) emission of light

   (c) desorption of light

   (d) scattering of light

7. The expression of Hamiltonian operator $\hat{H}$ is

   (a) $\frac{h^2}{8ma^2}\nabla^2 + V$

   (b) $-\frac{h^2}{8ma^2}\nabla^2 + V$

   (c) $\frac{h^2}{8ma^2}\nabla^2 - V$

   (d) $-\frac{h^2}{8ma^2}\nabla^2 - V$

8. In quantum mechanics, the quantity $|\psi|^2$ gives
   (a) volume of the system
   (b) density of the system
   (c) probability density
   (d) None of the above

9. According to the molecular orbital theory
   (a) the atomic orbitals interact leading to the formation of molecular orbitals
   (b) the number of molecular orbitals are equal to the number of combining atomic orbitals
   (c) electrons fill in the molecular orbitals on the same way as they fill the atomic orbitals
   (d) All of the above

10. According to Born-Oppenheimer approximation
   (a) the electrons in a molecule moves much faster than the nuclei
   (b) the Morse potential energy of a vibrating diatomic molecule is parabolic
   (c) the angular velocity of the electron is quantized
   (d) All of the above

(Continued)

SECTION—II

(*Marks* : 15)

Answer the following questions briefly : 2×5=10

1. What do you mean by electromagnetic spectrum?

2. Write a note on quenching of fluorescence.

3. State Franck-Condon principle.

4. Write the Schrödinger wave equation for hydrogen atom in spherical polar coordinates.

5. What happens when Hamiltonian operator is operated on a wave function?

Write True or False of the following : 1×5=5

6. The quantum yield of a photochemical process is defined as the number of molecules reacting in a given time per number of quanta of radiation absorbed in the same time.

7. Overtones in molecular spectroscopy arise due to anharmonic vibrations.

(Turn Over)

8. Bathochromic or red shift results in shorter wavelength.

9. The probability density can never be negative.

10. In quantum mechanics, quantization of energy arises naturally from the boundary condition.

(PART : B—DESCRIPTIVE)

(*Marks* : 50)

1. *(a)* Write the postulates of quantum mechanics. 4

(b) Derive the time independent Schrödinger wave equation. 3

(c) Normalize the wave function

$$\psi = A \sin \frac{n\pi x}{L}$$ 3

Or

2. *(a)* Derive the expression for the wave function ψ and total energy E for a particle of mass m in a box of length L moving in one dimension. 5

(b) What do you mean by quantization of energy? Explain why quantization of energy occurs in a particle in a box system but not in free particle system. 2+3=5

3. *(a)* Discuss the LCAO-MO treatment of $H_2^{\pm}$ molecular ion. 5

(b) Separate the variables r, Θ and Φ from Schrödinger wave equation for H-atom. 5

Or

4. *(a)* For H-atom, show that

$$E_n = -\frac{13 \cdot 6}{n^2} \text{ eV}$$ 3

(b) Write the difference between bonding and anti-bonding molecular orbitals. 3

(c) Give the common features and differences between MOT and VBT. 4

5. *(a)* Explain briefly the different types of molecular spectra. 5

(b) Discuss the relative intensities of rotational spectral lines. 3

(c) Write a short note on singlet and triplet states. 2

Or

6. *(a)* What do you mean by degrees of freedom of a molecule? Taking specific examples, explain the different types of degrees of freedom possessed by a linear and a non-linear molecule. 1+3=4

(b) Derive the expression for the force constant of a simple harmonic oscillator. 3

(c) Show diagrammatically the various electronic transitions of a polyatomic molecule. 3

7. *(a)* State and explain the Beer-Lambert law. 4

(b) Derive an expression for the photo-chemical equilibrium constant for a first-order reaction in which the forward reaction is a photochemical reaction and the backward reaction is a thermal reaction. 3

(c) What is photochemistry? How do the photochemical reactions differ from the thermal reactions? 1+2=3

Or

8. *(a)* State the Grotthuss-Draper law. What is the molar extinction coefficient? 1+1=2

(b) What are photochemical reactions? Explain the primary and secondary processes of photochemical reactions. 1+3=4

(c) Write a note on the difference between fluorescence and phosphorescence. Give one application each of fluorescence and phosphorescence. 2+2=4

9. *(a)* Derive the Schrödinger wave equation for one-dimensional simple harmonic oscillator. 4

(b) Discuss the formation of H_2 molecule from Valence Bond theory. 4

(c) Write a short note on Morse potential curve. 2

Or

10. *(a)* Explain the conditions for normalization and orthogonality of wave functions. 2+2=4

(b) From the LCAO-MO theory, construct the Schrödinger wave equation for H_2 molecule. 3

(c) What are photosensitizers? Write a note on chemiluminescence. 1+2=3

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