2025

(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

(PART : B—DESCRIPTIVE)

(*Marks* : 50)

The figures in the margin indicate full marks for the questions

1. *(a)* Derive the Schrödinger equation for a particle in one-dimensional box. 4

(b) Calculate the ground state energy (in eV) for an electron that is confined to a one-dimensional infinite potential well with a width of 0·2 nm. 3

(c) What are wave functions? Give the physical significance of wave function. 1+2=3

OR

2. *(a)* State and explain the Heisenberg uncertainty principle. 4

(b) Derive the Schrödinger equation in the form

$$\hat{H}\psi = E\psi$$ 4

(c) Write the expressions for the following : 1×2=2

(i) Normalized wave function

(ii) Orthogonal wave function

3. *(a)* Write the basic principles of molecular orbital theory (MOT). 3

(b) Discuss the application of LCAO-MO theory to study the H_2 molecule. 4

(c) Derive the Schrödinger equation for H-atom in spherical coordinates. 3

OR

4. *(a)* Discuss the application of valence bond theory (VBT) to H_2 molecules. 5

(b) Show how the average distance of electron from nucleus is calculated. 3

(Continued)

(c) Define bonding and antibonding molecular orbitals. 2

5. *(a)* Define fluorescence and phosphorescence with examples. 3

(b) Discuss the principle of NMR spectroscopy. 4

(c) Explain Born-Oppenheimer approximation. 3

OR

6. *(a)* Discuss the factors influencing vibrational frequencies. 4

(b) Explain the following terms : 3×2=6

(i) Chemical shift

(ii) Spin-spin interaction

7. *(a)* State and explain the Stark-Einstein law of photochemical equivalence. 4

(b) Calculate the number of moles of HCl(g) produced by the absorption of 1 J of radiant energy of wavelength 480 nm in the reaction $H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$ if the quantum yield of the photochemical reaction is $1{\cdot}0\times10^6$. 3

(c) Define photochemical equilibrium with an example. 3

(Turn Over)

OR

8. *(a)* What is quantum yield? Explain an example of low quantum yield reaction. 1+3=4

(b) A 0·005 *M* aqueous solution of a certain substance absorbs 15% of the incident light in a Beer-Lambert law cell of path length 2 cm. Calculate the concentration required for 90% absorption of the incident light. 3

(c) Discuss the importance of quenching in photochemical reactions. 3

9. *(a)* What is the significance of isotopic substitution in rotational spectroscopy? 3

(b) Write the similarities between valence bond theory (VBT) and molecular orbital theory (MOT). 3

(c) What are radial probability distribution curves? Explain with appropriate diagram. 1+3=4

OR

10. *(a)* Discuss the following types of molecular spectra : 2×2=4

(i) Rotational spectra

(ii) Electronic spectra

(Continued)

(b) Derive the mathematical form of Lambert-Beer law. 3

(c) What is an operator? When are the operators said to commute? 1+2=3

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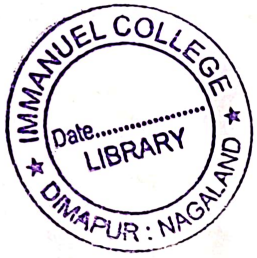

2025

(FYUGP)

(6th Semester)

CHEMISTRY

(MINOR)

Paper : CHEM.M–6 (T)

(Physical Chemistry—V : Quantum Chemistry and Spectroscopy)

(PART : A—OBJECTIVE)

(*Marks* : 25)

The figures in the margin indicate full marks for the questions

SECTION—I

(*Marks* : 10)

Put a Tick (✓) mark against the correct answer in the brackets provided : 1×10=10

1. According to Heisenberg's uncertainty principle, if the position of a particle is precisely known, then

   (a) its momentum is also precisely known ( )

   (b) its momentum is completely uncertain ( )

   (c) its energy is precisely known ( )

   (d) its velocity is zero ( )

2. The probability of finding a particle in a certain region is given by

(a) ψ ( )

(b) $|\psi|^2$ ( )

(c) $\int \psi \, dx$ ( )

(d) $P = mV$ ( )

3. In molecular orbital theory, bonding molecular orbitals

(a) decrease electron density between nuclei ( )

(b) increase electron density between nuclei ( )

(c) have no electron density ( )

(d) are always unoccupied ( )

4. The most probable distance of an electron from the nucleus in a hydrogen atom corresponds to

(a) the Bohr radius ( )

(b) twice the Bohr radius ( )

(c) the nucleus itself ( )

(d) the ionization energy ( )

5. In rotational spectroscopy, selection rules state that a molecule must

(a) have a permanent dipole moment ( )

(b) be linear ( )

(c) have a non-zero vibrational frequency ( )

(d) be symmetric ( )

6. Which principle explains the intensity of electronic transition?

(a) Born-Oppenheimer approximation ( )

(b) Franck-Condon principle ( )

(c) Heisenberg uncertainty principle ( )

(d) Aufbau principle ( )

7. According to Beer-Lambert law, the absorbance is directly proportional to

(a) concentration of the absorbing species ( )

(b) wavelength of the incident light ( )

(c) temperature of the solution ( )

(d) pressure of the system ( )

8. Which of the following is an example of photosensitized reaction?

(a) Hydrogenation of alkanes ( )

(b) Photosynthesis ( )

(c) Acid-base neutralization ( )

(d) Precipitation reactions ( )

9. Which factor does not influence quantum yield?

(a) Presence of intermediates ( )

(b) Temperature of the system ( )

(c) Number of photons absorbed ( )

(d) Spin of the electron ( )

10. Which of the following conditions must a valid wave function (ψ) satisfy?

(a) It must be continuous ( )

(b) It must be single-valued ( )

(c) Its first derivative must be continuous ( )

(d) All of the above ( )

SECTION—II

(*Marks* : 10)

Answer any *five* of the following in not more than *5* sentences each : 2×5=10

1. What is a linear operator? Give example.

2. What are the drawbacks of valence bond theory (VBT)?

3. What is Morse potential?

4. What will happen if the walls of the one-dimensional box are suddenly removed?

5. State Grotthuss-Draper law.

6. What are overtones in vibrational spectroscopy?

7. What are photochemical reactions? Give examples.

SECTION—III

(*Marks* : 5)

Indicate *True (T)* or *False (F)* by putting a Tick (✓) mark. 1×5=5

1. The Schrödinger equation for a hydrogen atom is solved in Cartesian coordinates.

(*T* / *F*)

2. Bonding MO have lower energy than antibonding MO.

(*T* / *F*)

3. Phosphorescence occurs due to transition between singlet states.

(*T* / *F*)

4. In rotational spectroscopy, isotopic substitution does not affect the spectrum.

(*T* / *F*)

5. The Morse potential accounts for molecular bond dissociation.

(*T* / *F*)

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