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**1 (Sem-4/FYUGP) CHE 43 MJ**

**2026**

**CHEMISTRY**

**( Major )**

Paper : CHE4400304MJ

**( Theoretical Chemistry )**

Full Marks : 45

Time : 2 hours

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

1. Answer the following questions as directed :

1×5=5

(i) The operators used in quantum mechanics are

- (a) Real
- (b) Hamiltonian
- (c) Commutator
- (d) Linear

(ii) The dual nature of electron leads to the quantization of angular momentum of the electron in atomic orbitals.

(State whether the statement is True **or** False)

(iii) What are well behaved functions ?

(iv) What is the zero point energy of a linear harmonic oscillator ?

(v) Dispersion forces are present only in \_\_\_\_\_ .  
(Fill in the blank)

2. Answer **any five** from the following questions :

2×5=10

(i) What is the de Broglie hypothesis ?

(ii) What do you mean by eigenfunction and eigenvalue ?

(iii) What is the physical significance of  $\psi$  ?

(iv) Write the expression for the radial wave function for hydrogen like atom.

(v) What is nodal plane ? How many nodal planes are there in  $3p$  orbital ?

(vi) If  $\hat{A} = 3x^2$  and  $\hat{B} = \frac{d}{dx}$ , show that  $\hat{A}$

and  $\hat{B}$  do not commute.

(vii) For a particle in a cubical box, determine the degree of degeneracy of the energy level (a)  $14h^2/8ma^2$  and (b)  $9h^2/8ma^2$ .

(viii) A particle is confined in a one dimensional box of length  $a$  where potential energy is zero. Calculate the probability of finding the particle within the interval  $0 \leq x \leq a/2$ .

(ix) Explain why  $s$  orbital is spherically symmetric.

(x) Write a note on dipole moment and molecular structure.

3. Answer **any four** from the following questions :  $5 \times 4 = 20$

(i) What is Hermitian operator? Prove that the eigenvalues of hermitian operators are real.  $2+3=5$

(ii) What are linear and commutator operator? Verify whether the operators  $\hat{A}$  and  $\hat{B}$  commute or not if

(a)  $\hat{A} = 3x^2$  and  $\hat{B} = \frac{d}{dx}$

(b)  $\hat{A} = \frac{d}{dx}$  and  $\hat{B} = \frac{d^2}{dx^2} + 2 \frac{d}{dx}$   
 $2+1\frac{1}{2}+1\frac{1}{2}=5$

(iii) What is the ground state energy of a particle confined in a one dimensional box? Find the ground state energy of an electron confined in a one dimensional box of  $20\text{\AA}$ .

What will be the frequency of the emitted radiation when the electron undergoes transition from  $n=2$  level to  $n=1$  level?  $1+2+2=5$

(iv) What do you mean by orbital? Describe the shapes of  $s$ ,  $p$  and  $d$  orbitals.  $1+4=5$

(v) Compare the Valence Bond Theory with Molecular Orbital Theory.

(vi) Using Born Oppenheimer Approximation explain the potential energy curve for  $H_2^+$  ion.

(vii) What is meant by polarizability of a molecule? Describe the Clausius-Mossotti Equation.  $1+4=5$

(viii) Explain the terms electronic polarization, atomic polarization and orientation polarization. Give *two* examples of polar molecules.  $3+2=5$

4. Answer **any one** from the following questions :  $10 \times 1 = 10$

(i) (a) Explain Photo Electric Effect. 5

(b) The work function of Cesium metal is  $2.14\text{eV}$ . Calculate the kinetic energy and the speed of electrons when the metal is irradiated with a light of wave length (i)  $550\text{nm}$ , (ii)  $400\text{nm}$ .  $2\frac{1}{2}+2\frac{1}{2}=5$

(ii) (a) Set up and solve the Schrödinger wave equation for a particle of mass  $m$  moving in a one dimensional box with rigid walls of width  $a$ . 5

- (b) What do you mean by expectation value of a measurable quantity? Show that for a particle in one dimensional box of width  $a$ ,

(i)  $\langle x \rangle = a/2$ , (ii)  $\langle P_x \rangle = 0$ .

$$2 + 1\frac{1}{2} + 1\frac{1}{2} = 5$$

- (iii) (a) Show that the following radial wave function of hydrogen atom is normalized :

$$R_{1,0}(r) = (2/a_0)^{3/2} \exp(-r/a_0) \quad 3$$

- (b) What is the most probable distance of the electron of hydrogen atom in its  $2p$  state.

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- (c) Calculate the zero point energy of a simple harmonic oscillator with frequency  $40\text{Hz}$ .

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- (d) Determine the ground state term symbol for the ground state of the atoms with outer electronic configuration : (i)  $2p^2$  and (ii)  $3d^8$ .

$$1\frac{1}{2} + 1\frac{1}{2} = 3$$

- (iv) (a) Write the Schrödinger wave equation for Hydrogen atom in terms of polar co-ordinates. 2

- (b) What are radial probability distribution curves? Discuss it for  $2s$  and  $3s$  orbitals.

$$1 + 2 = 3$$

- (c) Solve the Schrödinger equation for  $H_2^+$  ion.

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