Total number of printed pages–7

1 (Sem–4/FYUGP) CHE 43 MJ

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Acc. No.
Date
Nagaon : Assam

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 ψ ?

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

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

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3. Answer ***any four*** from the following questions : 5×4=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+1½+1½=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 20Å..

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

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(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 : 10×1=10

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

(b) The work function of Cesium metal is 2·14*eV*. Calculate the kinetic energy and the speed of electrons when the metal is irradiated with a light of wave length (i) 550*nm*, (ii) 400*nm*. 2½+2½=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+1½+1½=5

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

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

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

(c) Calculate the zero point energy of a simple harmonic oscillator with frequency 40*Hz*. 2

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

1½+1½=3

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

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(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. 5