2024/12

**SET A**

# M.Sc. CHEMISTRY
## FIRST SEMESTER
## QUANTUM CHEMISTRY-I
## MSC – 104 [REPEAT]

[USE OMR FOR OBJECTIVE PART]

**Duration: 1:30 hrs.** **Full Marks: 35**

## Objective

**Time: 15 mins.** **Marks: 10**

***Choose the correct answer from the following:*** ***1×10=10***

1. What is the commutator of two Hermitian operators A and B?
   a. [A, B] = AB
   b. [A, B] = 0
   c. [A, B] = BA
   d. [A, B] = A + B

2. In quantum mechanics, what physical quantity is associated with a non-commutative pair of Hermitian operators?
   a. Position and momentum
   b. Spin components
   c. Energy and time
   d. Angular momentum

3. Which of the following is a necessary condition for an operator to be Hermitian?
   a. It has real eigenvalues
   b. It commutes with all other
   c. Its adjoint is equal to itself
   d. It is a linear operator

4. What is the commutation property of a Hermitian operator with its own adjoint?
   a. [A, A†] = 0
   b. [A, A†] = AA†
   c. [A, A†] = A†A
   d. [A, A†] = A

5. The eigenstates of an operator correspond to:
   a. States with definite values of the observable associated with that operator
   b. A probability distribution.
   c. States of definite energy.
   d. States of definite position.

6. What is the potential energy term in the Schrodinger equation for a particle outside the boundaries of a confined one-dimensional box?
   a. V = 0
   b. V = ∞
   c. V = 1
   d. V = -1

7. What is the solution to the Schrodinger equation for a particle lying outside the boundaries of a confined one – dimensional box?
   a. $\Psi_n(x) = 0$
   b. $\Psi_n(x) = \infty$
   c. $\Psi_n(x) = 1$
   d. $\Psi_n(x) = -1$

8. The number of nodes in the wavefunction plot for a particle in one – dimensional box is given by (where n is a quantum number)

a. n
b. n+1
c. n-1
d. n+2

9. The ground state energy for a simple harmonic oscillator in a three-dimensonal cubic box is

a. $3h\upsilon$
b. $\frac{1}{2}h\upsilon$
c. $2h\upsilon$
d. $\frac{3}{2}h\upsilon$

10. Which of the following relation is correct?

a. $e^{i2m\pi} = cos2m\pi - isin2m\pi$
b. $e^{i2m\pi} = sin2m\pi - icos2m\pi$
c. $e^{i2m\pi} = cos2m\pi + isin2m\pi$
d. $e^{i2m\pi} = sin2m\pi + icos2m\pi$

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# Descriptive

**Time : 1 hr. 15 mins.** **Marks: 25**

***[ Answer question no.1 & any two (2) from the rest ]***

1. **a.** Write the expressions for the Schrodinger equation for a particle inside and outside of one – dimensional box. **3+2=5**

   **b.** What is the commutation value of $(\frac{d}{dx} - x)^2$ ?

2. **a.** Sketch the wavefunctions of a particle in a one-dimensional box for n = 1, 2, and 3 with the evaluation of the x-axis coordinates. **6**

   **b.** Write the energy expression for a simple harmonic oscillator in a three-dimensonal cubic box. What do you meant by degeneracy of a state? Explain degeneracy for a simple harmonic oscillator in a three-dimensonal cubic box. **1+1+2=4**

3. **a.** Write down the Schrodinger equation for a particle on a ring. Find out the expressions of eigenvalue and normalized eigenfunction of the Schrodinger equation for a particle on a ring. **1+4=5**

   **b.** What is the zero point energy for the particle on a ring? Explain briefly why all energy levels are doubly degenerate except the lowest one for the particle on a ring? **1+2=3**

   **c.** What do you mean by quantum mechanical tunneling? Explain. **2**

4. **a.** Find the acceptable wave functions: $\sqrt{x}$ and $e^{-\infty}(-\infty,\infty)$ **2+2+3+1+2=10**

   **b.** Find if the operators of position & momentum commute or not?

   **c.** Write about the different properties of commutator.

d. Find the commutation value of $[k P_z, m Z^n]$. (Where, k & m are constants)

e. Find the commutation value of $[x^2, [x, p_x^2]]$.

5. a. The Value of commutation of $d/dx$ with $d^2/dx^2 + 2(d/dx)$ is? 1+2+2+3+2=10

b. Find the commutation value of angular momentum with position & angular momentum with linear momentum.

c. If, A and B are hermitian, Find which of these are hermitian?
**AB, ABA, i[A,B] , and $A^2B$**

d. Derive the Schrodinger's Wave Equation for a particle in a 1-D box of length '*l*' and write one application of it.

e. Prove that $P_x$ is hermitian. (Where, $P_x$ is momentum operator)

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