REV-01
MSC/05/10

2024/07

**SET A**

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

[USE OMR SHEET FOR OBJECTIVE PART]

**Duration : 1.30 hrs.** **Full Marks : 35**

**( Objective )**

**Time: 15 min.** **Marks: 10**

***Choose the correct answer from the following:*** ***1X10=10***

1. The normalization constant for a particle in 1D box in between length 0 to l with wavefunction $\Psi = \sin\left(\frac{n\pi x}{l}\right)$ is

   a. $\sqrt{\frac{2}{l}}$ b. $\sqrt{\frac{2!}{x}}$

   c. $\sqrt{\frac{1}{x}}$ d. $\sqrt{\frac{l}{4}}$

2. What is the eigenvalue of $\frac{d}{dx}(e^{ax})$

   a. $e^{ax}$ b. a

   c. 1/a d. Not an eigenvalue equation

3. The value of the commutator of $\hat{x}$ with $\hat{p_x}$ is

   a. ih b. -ih

   c. - h d. h

4. The time independent Schrodinger's equation of a system represents the conservation of the

   a. Total binding energy of the system b. Total potential energy of the system

   c. Total kinetic energy of the system d. Total energy of the system

5. The degeneracy of the n=2 level for a three-dimensional isotropic oscillator is___.

   a. 3 b. 6

   c. 9 d. 2

6. The acceptable wavefunction is

   a. Ψ=sin x b. Ψ=tan x

   c. Ψ=x d. Ψ=cosec x

7. The operator $\nabla^2$ is called _____operator

   a. Hamiltonian b. Laplacian

   c. Adjoint d. Hermitian

8. For the adjoint of the product of two operators A and B, $(AB)^{\dagger}$=____

a. $B^{\dagger}A^{\dagger}$ b. AB

c. $A^{\dagger}B^{\dagger}$ d. 1

9. If $\delta_{mn}$ is Knocker delta function then $\delta_{mn} = 0$ when ____

a. m=n b. m>n

c. m<n d. m≠n

10. Angular momentum is defined as

a. $\vec{r}\times\vec{p}$ b. $\vec{r}\times\vec{p}^{2}$

c. $\vec{r}.\vec{p}$ d. mv

-- --- --

# Descriptive

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

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

1. Derive and solve the Schrodinger wave equation for a particle in a one-dimensional box. 5

2. **a.** Derive and solve the Schrodinger wave equation for rigid rotor. 5+3+2 =10

   **b.** The lowest energy of a quantum mechanical one-dimensional simple harmonic oscillator is 300 $cm^{-1}$. What is the energy (in $cm^{-1}$) of the next higher level?

   **c.** Define Hermitian operator.

3. **a.** What is degeneracy? Give the degeneracy of a 3D box with energy $E = \frac{n^2 h^2 \pi^2}{2ma^2}$ 4+6=10

   **b.** What are normalized, orthogonal and orthonormal wavefunctions?

4. **a.** Calculate the average value of the position <x> for a particle in a one-dimensional box of width 'a'. 3+5+2 =10

   **b.** Derive and solve the Schrodinger wave equation for particle in a ring.

   **c.** What is eigenfunction and eigenvalue?

5. **a.** Evaluate $[\hat{L}_-, \hat{L}_z]$ 2+3+5 =10

   **b.** What is the restriction on $\alpha/\beta$ if the n=1 wavefunction of a one-dimensional SHO has to satisfy the wavefunction $\frac{d^2\Psi}{d\xi^2} + \left(\frac{\alpha}{\beta} - \xi^2\right)\Psi = 0$? Given that $\Psi = N\xi \exp\left(-\frac{\xi^2}{2}\right)$ where N is a constant.

   **c.** State the postulates of quantum chemistry.

= = *** = =