

M.Sc. CHEMISTRY
FIRST SEMESTER
QUANTUM CHEMISTRY-I
MSC – 104 IDMn

[USE OMR SHEET FOR OBJECTIVE PART]

**SET
A**

Duration : 1.30 hrs.

Full Marks : 35

Time: 15 min.

(Objective)

Marks: 10

1X10=10

Choose the correct answer from the following:

1. The acceptable wavefunction is

a. $\Psi = \sin x$
c. $\Psi = x$

b. $\Psi = \tan x$
d. $\Psi = \operatorname{cosec} x$

2. The phase velocity of a particle moving with a velocity v is

a. $\frac{c}{v}$
c. $\frac{v^2}{c}$

b. $\frac{c^2}{v}$
d. $\frac{v}{c}$

3. The de-broglie wavelength of a particle of mass 'm' and kinetic energy E_k is

a. $\frac{h}{2mE_k}$
c. $\frac{h}{\sqrt{2mE_k}}$

b. $\frac{h}{2m\sqrt{E_k}}$
d. $\frac{h}{\sqrt{mE_k}}$

4. Which of the following is an eigenvalue equation of operator $\hat{\lambda}$ and eigenvalue λ ?

a. $\hat{\lambda}\Psi = \lambda\phi$

b. $\hat{\lambda}\Psi = \frac{1}{\lambda}\phi$

c. $\hat{\lambda}\Psi = \frac{1}{\lambda}\Psi$

d. $\hat{\lambda}\Psi = \lambda\Psi$

5. Which of the following is correct?

a. $\hat{x}\hat{p}_x - \hat{p}_x\hat{x} = \frac{\hbar}{i}$

b. $\hat{x}\hat{p}_x - \hat{p}_x\hat{x} = \frac{h}{i}$

c. $\hat{x}\hat{p}_x - \hat{p}_x\hat{x} = -\frac{\hbar}{i}$

d. $\hat{x}\hat{p}_x - \hat{p}_x\hat{x} = -\frac{h}{i}$

6. 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. $\sqrt{\frac{2}{l}}$
c. $\sqrt{\frac{2l}{x}}$

b. $\sqrt{\frac{2l}{x}}$
d. $\sqrt{\frac{l}{4}}$

7. The Hamiltonian for a rigid rotor is given by

- a. 0
b. $\frac{L^2}{2I}$ ✓
c. $\frac{I^2}{2L}$
d. $\frac{2L}{I^2}$

8. The value of Hermite polynomial $H_1(\xi)$ is given by

- a. 1
b. $4\xi^2 - 2$
c. 2ξ ✓
d. 0

9. If $\phi = Ae^{im\phi}$, then value of A after normalization is

- a. $\frac{1}{\sqrt{\pi}}$
b. $\frac{1}{\sqrt{2\pi}}$ ✓
c. $\frac{1}{\sqrt{3\pi}}$
d. $\frac{2}{\sqrt{\pi}}$

10. The degeneracy of the n=2 level for a three-dimensional isotropic oscillator is ____.

- a. 3
b. 6 ✓
c. 9
d. 2

(Descriptive)

Time : 1 hrs. 15 mins.

Marks : 25

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

- a. Calculate the average value of the position (x) for a particle in a box of length 'a'. 3+2=5
- b. What is quantum tunnelling effect?
2. a. State the postulates of quantum mechanics. 5+5=10
- b. Define Hermitian operator and prove that the eigenvalue of Hermitian operator is real.
3. a. Starting from the definition of L_+ and L_- find the value of $[L_+, L_-]$ 5+5=10
- b. Prove that eigenfunctions of a Hermitian operator corresponding to different eigenvalues are orthogonal.
4. a. What is degeneracy? Give the degeneracy of a 3D box with energy 4+6=10
- $$E = \frac{27 h^2 v^2}{2 m a^2}$$
- b. Derive and solve the Schrodinger wave equation for rigid rotor
5. a. Derive and solve the Schrodinger wave equation for a particle in a ring. 6+4=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?

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