

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

**SET
A**

[USE OMR SHEET FOR OBJECTIVE PART]

Duration : 1.30 hrs.

Full Marks : 35

Time: 15 min.

(Objective)

Marks: 10

Choose the correct answer from the following:

1X10=10

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

- b. $\hat{\lambda}\Psi = \frac{1}{\lambda}\Phi$
d. $\hat{\lambda}\Psi = \lambda\Psi$

5. Which of the following is correct?

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

- b. $\hat{x}\hat{p}_x - \hat{p}_x\hat{x} = \frac{h}{i}$
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 1 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]

1. 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 \bar{L}_+ and \bar{L}_- find the value of $[\bar{L}_+, \bar{L}_-]$ 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

$$E = \frac{27 h^2 \pi^2}{2m a^2}$$

 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?

= = *** = =