CHEMICAL SCIENCES (NET-JRF/GATE)

Unit Test: Quantum Chemistry

Time : 00: 50 Hour **Batch-I** **Date : 04-02-2014**
M.M. : 50

Instructions:

1. **Question Paper contains 25 objective type questions, each question carry 2 marks.**
2. **There is negative marking, 0.5 mark will be deducted for each wrong answer**
3. **Attempt all the questions, use of calculator is not allowed.**

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1. For Eigen function $\frac{1}{\pi}\sin 3.63x$, the eigenvalue of operator $\frac{-h^2}{8\pi^2 m}\frac{d^2}{dx^2}$ is :

(a) $\frac{(3.63)^2 h^2}{8\pi^3 m}$ (b) $\frac{(3.63)^2 h^2}{8\pi^2 m}$ (c) $\frac{-(3.63)^2 h^2}{8\pi^3 m}$ (d) $\frac{-(3.63)^2 h^2}{8\pi^2 m}$

2. For a particle in a one D box with infinite walls at x=0 and in the n = 3 state, the probability for finding the electron in the range $0 \le x \le \frac{L}{4}$ is:

(a) Greater than $\frac{1}{3}$ (b) Exactly $\frac{1}{6}$

(c) Exactly $\frac{1}{3}$ (d) None of the above is correct.

3. Which one of the following statement is true about the particle in 1D box with infinite wall.

(a) $\int \psi_3^2 dx = 0$ because these wavefunction are orthogonal.

(b) $\int \psi_1\psi_3 dx = 0$ because both these function are symmetric.

(c) $\int \psi_1\psi_2 dx = 0$ because these wavefunction are normalised.

(d) $\int \psi_1\psi_3 dx = 0$ because these wavefunction are orthogonal.

4. Which of the following is true

(a) $[L_x, x] = 0$; $[L_x, p_x] = 0$; $[x, p_x] = 0$

(b) $[L_x, L_y] = i\hbar L_z$; $[L_x, y] = i\hbar p_z$; $[y, p_x] = 0$

(c) $[x, y] = 0$; $[L^2, L_x] = 0$; $[y, p_y] = 0$

(d) $[L_x, L_z] = -i\hbar L_y$; $[y, p_x] = 0$; $[L_x, x] = 0$

5. Consider a quantum mechanical problem where the eigenfunction is the spherical harmonic

$$Y_{\ell m} \text{ with } \ell = 1 \text{ and } m_1 = 0, \text{ i.e. } Y_{10}(\theta, \phi) = N\cos\theta$$

Find the normalization constant N.

(a) $\sqrt{3/6\pi}$ (b) $\sqrt{3/2\,\pi}$ (c) $\sqrt{3/\pi}$ (d) $\sqrt{3/4\,\pi}$

6. Given two hermitian operator A and B, we construct the following four additional operator.

$$AB,\ ABA,\ i[AB],\ A^2B$$

Choose the correct option from below.

(a) All the 4 operator are hermitian
(b) Only 3 of these operator are hermitian.
(c) Only 2 of these operator are Hermitian
(d) Only 1 of operator is hermitian.

7. Which of the following pairs of operator commute?

(a) x^2 and $\frac{d}{dx}$
(b) x^3 and $\frac{d^2}{dx^2}$
(c) $\frac{d^2}{dx^2}$ and $\frac{d}{dx}+2\frac{d^2}{dx^2}$
(d) $x^2\frac{d}{dx}$ and $\frac{d^2}{dx^2}$

8. Consider the following statement:
(1) All eigenvalues are real.
(2) Eigenfunction of Hamiltonian operator are orthogonal to each other.
(3) Two Hermitian operator A and B commute and A and B are Hermitian. Separately than AB is also Hermitian.
(4) The eigenvalue of anti Hermitian are either purely imaginary or equal to zero
Which of these are true

(a) 1, 2, 3
(b) 1, 3, 4
(c) 2, 3
(d) 1, 2, 3, 4

9. Consider a free particle of mass m moving in one dimension . Than $[\hat{H}, x] =$
(Where H and x are Hamiltonian and momentum operator)

(a) $\frac{-ih}{2\pi}\frac{\hat{p}}{m}$
(b) $i\hbar\frac{\hat{p}}{m}$
(c) $\frac{h}{2\pi}\frac{\hat{p}}{m}$
(d) $-\frac{h}{2\pi}\frac{\hat{p}}{m}$

10. Given two hermitian operator A and B. We construct the following three additional operator.

AB or $A^2B,\ AB^2$
ABA

Choose the correct option as below

(a) All these four operator are hermitian.
(b) Only 3 of these are hermitian.
(c) Only two of these are hermitian
(d) Only one of the operator is hermitian.

11. A electron of mass 'm' is confined to a one dimensional box of length 2b. It makes a radiative transition from 3^{rd} excited state to ground state then, the frquency of transtion

(a) $\frac{15h}{32mb^2}$
(b) $\frac{15h}{9mb^2}$
(c) $\frac{h}{8\,mb^2}$
(d) $\frac{h}{32\,mb^2}$

12. The second excited state wave function of a particle between $-\frac{\ell}{2}$ to $+\frac{\ell}{2}$ is:

(a) $\sqrt{\frac{2}{\ell}}\cos\frac{3\pi x}{\ell}$
(b) $\sqrt{\frac{2}{\ell}}\cos\frac{3\pi x}{2\ell}$
(c) $\sqrt{\frac{1}{\ell}}\cos\frac{3\pi x}{2\ell}$
(d) $\sqrt{\frac{1}{\ell}}\cos\frac{3\pi x}{\ell}$

13. $[L_x, L_y]$ and $[L_x, y]$ is respectively

(a) $-i\hbar L_z, \frac{h}{2\pi i}z$
(b) $\frac{i\hbar}{2\pi}L_z, i\hbar z$
(c) $-\frac{h}{2\pi i}L_z, i\hbar z$
(d) $\frac{h}{2\pi i}L_z, i\hbar z$

14. An operator A is defined as $A = -\frac{d}{dx} + ix$. Then

(a) A is hermitian (b) A is antihermitian

(c) $AA^\dagger$ and $AA^\dagger$ are antihermitian (d) None of these

15. The wave function for a quantum mechanical particle in a one dimensional box of length 'a' is given by $\psi = A\sin\frac{2\pi x}{a}$. The value of A for a box of length 100 nm is:

(a) $.141\ nm^{-1/2}$ (b) $.282\ nm^{-1/2}$ (c) $10\sqrt{2}\,(nm)^{-1/2}$ (d) $0.1\,(nm)^{-1/2}$

16. If the $\psi_{n,\ell,m}$ are the eigenfunction of the operator $L_x^2 + L_y^2$ then what is the eigenvalue.

(a) $\ell(\ell+1)\hbar^2$ (b) $m\ell^2\hbar^2$ (c) $\ell(+1)\hbar^2 + m^2\hbar^2$ (d) $\ell(\ell+1)\hbar^2 - m^2\hbar^2$

17. A particle is moving in one dimension between x = a and x = b. The potential energy is such that the particle can not be outside these limit and the wave function in between is $\psi = \frac{A}{x}$. The average value of x is:

(a) $\sqrt{\frac{ab}{b-a}}$ (b) $\sqrt{\frac{ab}{b-a}}\ell n\frac{b}{a}$ (c) $\frac{ab}{b-a}\ell n\frac{b}{a}$ (d) $\sqrt{\frac{ab}{b-a}}\ell n\frac{a}{b}$

18. The commutator $\left[x^2, p^2\right]$ is

(a) $2\,i\hbar\,xp$ (b) $2i\hbar(xp+px)$ (c) $2i\hbar px$ (d) $2i\hbar(xp-px)$

19. The electronic wavefunction $\langle\psi\rangle$ for hydrogen atom in 2s state is $\psi\alpha\left(2-\frac{r}{a_0}\right)e^{-\frac{r}{2a_0}}$, than the value of $\langle r\rangle$ is:

(a) $\frac{3}{2}a_0$ (b) $6a_0$ (c) $2a_0$ (d) None of these

20. The probability of finding the electron between 0 to $2a_0$ for 1s orbital of H-atom.

$$R_{1s} = \frac{2}{a_0^{3/2}}e^{-r/a_0}$$

(a) 32% (b) 76% (c) 64% (d) 84%

21. For the particle in box problem in (0, L). The value of $\left\langle x^3\right\rangle$ in the $n \to \infty$ limit would be

(a) $\frac{L^3}{6}$ (b) $\frac{L^3}{3}$ (c) $\frac{L^3}{4}$ (d) $\frac{L^4}{4}$

22. Operator $\left[x,\left[x, p^2\right]\right]$ is identical with

(a) $\left[p_x,[x,p]\right]$ (b) $\left[x_p,[x,p]\right]$ (c) $-\left[p,\left[x^2,p\right]\right]$ (d) $\left[x\left[x^2,p\right]\right]$

23. An electron in a one-dimensional infinite well, defined by $V(x)=0$ for $-a \le x \le a$ and $V(x)=\infty$ otherwise, goes from the $n=4$ to the $n=2$ level. The frequency of the emitted photon is 3.43×10^{14} Hz. Find the width of the box.

(a) $8.92\times10^{-10}\,m$
(b) $17.84\times10^{-10}\,m$
(c) $4.46\times10^{-2}\,m$
(d) None of thes

24. The quantum-mechanical probability of finding the particle in a one-dimensional 'box' in the middle third of the 'box' for first excited state is:

(a) 0.20 (b) 0.40 (c) 0.60 (d) 0.33

25. Three real function ψ_1, ψ_2 and ψ_3 are normalised and orthogonal normalize constant of the wave function

$$Z=\psi_1-\frac{1}{\sqrt{2}}\psi_2+\frac{\sqrt{3}}{\sqrt{2}}\psi_3 \text{ is}$$

(a) $\frac{1}{\sqrt{3}}$ (b) $\frac{1}{\sqrt{6}}$ (c) $\frac{1}{\sqrt{2}}$ (d) $\frac{\sqrt{3}}{\sqrt{2}}$

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[ANSWERS]

1. (b)	2. (d)	3. (d)	4. (d)	5. (d)	6. (c)	7. (c)
8. (d)	9. (a)	10. (d)	11. (a)	12. (a)	13. (c)	14. (d)
15. (a)	16. (d)	17. (c)	18. (b)	19. (b)	20. (b)	21. (c)
22. (c)	23. (b)	24. (a)	25. (a)			