CHE 502

M.Sc. Ist SEMESTER EXAMINATION, 2022-23

CHEMISTRY

(Quantum Chemistry -I)

(4+0)

(CBCS MODE)

AFFIX PRESCRIBED RUBBER STAMP

Date (तिथि) : ____________

Paper ID
(To be filled in the OMR Sheet)

8402

अनुक्रमांक (अंकों में) :
Roll No. (In Figures)

अनुक्रमांक (शब्दों में) : ____________

Roll No. (In Words) : ____________

Time : 1 Hour | **Max. Marks : 60**
समय : 1 घण्टा | अधिकतम अंक : 60

नोट : पुस्तिका में 40 प्रश्न दिये गये हैं, सभी प्रश्न करने होंगे। प्रत्येक प्रश्न 1.5 अंक का होगा।

Important Instructions :

1. The candidate will write his/her Roll Number only at the places provided for, i.e. on the cover page and on the OMR answer sheet at the end and nowhere else.

2. Immediately on receipt of the question booklet, the candidate should check up the booklet and ensure that it contains all the pages and that no question is missing. If the candidate finds any discrepancy in the question booklet, he/she should report the invigilator within 10 minutes of the issue of this booklet and a fresh question booklet without any discrepancy be obtained.

महत्वपूर्ण निर्देश :

1. अभ्यर्थी अपने अनुक्रमांक केवल उन्हीं स्थानों पर लिखेंगे जो इसके लिए दिये गये हैं, अर्थात् प्रश्न पुस्तिका के मुख्य पृष्ठ तथा साथ दिये गये ओ०एम०आर० उत्तर पत्र पर, तथा अन्यत्र कहीं नहीं लिखेंगे।

2. प्रश्न पुस्तिका मिलते ही अभ्यर्थी को जाँच करके सुनिश्चित कर लेना चाहिए कि इस पुस्तिका में पूरे पृष्ठ हैं और कोई प्रश्न छूटा तो नहीं है। यदि कोई विसंगति है तो प्रश्न पुस्तिका मिलने के 10 मिनट के भीतर ही कक्ष परिप्रेक्षक को सूचित करना चाहिए और बिना त्रुटि की दूसरी प्रश्न पुस्तिका प्राप्त कर लेना चाहिए।

1. If Ψ_i and Ψ_j are the two acceptable wave functions of a given system, then these wave functions are said to be orthogonal if :

(A) $\int \Psi_i \Psi_j \, d\tau = 0$

(B) $\int \Psi_i \Psi_j \, d\tau = 1$

(C) $\int \Psi_i \Psi_j \, d\tau = \infty$

(D) None of these

2. Schrodinger wave equation in terms of Laplacian operator may be written as :

(A) $\hat{H} \Psi = E \Psi$

(B) $\nabla^2 \Psi - \frac{8\pi^2 m(E-V)}{h^2} \Psi = 0$

(C) $\nabla^2 \Psi + \frac{8\pi^2 m(E-V)}{h^2} \Psi = 0$

(D) $\nabla^2 \Psi + \frac{8\pi^2 m}{h^2} \Psi = 0$

3. If Ψ_1 and Ψ_2 are the Eigen functions of the operator $\hat{A}$, then the operator $\hat{A}$ is said to be Hermitian operator if :

(A) $\int \Psi_1^* (\hat{A} \Psi_2) \, d\tau = \int (\hat{A} \Psi_1)^* \Psi_2 \, d\tau$

(B) $\int \Psi_1 \hat{A} \Psi_2 \, d\tau = \int \Psi_2 \hat{A} \Psi_1 \, d\tau$

(C) $\int \Psi_1^* \hat{A} \Psi_2 \, d\tau = \int \Psi_1 \hat{A} \Psi_2^* \, d\tau$

(D) None of these

4. The perturbed Hamiltonian $(\hat{H})$ can be expressed as $\hat{H} = \hat{H}^o + \lambda \hat{H}'$

Where $\lambda H'$ is the amount of perturbation :

(A) If $\hat{H}^o$ is the Hamiltonian of the unperturbed state

(B) If $\hat{H}^o$ is the Hamiltonian of the perturbed state

(C) (A) and (B) both

(D) None of these

5. An acceptable wave function, Ψ of a given system is said to be normalized, if :

(A) $\int \Psi^2 \, d\tau = 0$

(B) $\int \Psi^2 \, d\tau = \infty$

(C) $\int \Psi^2 \, d\tau = 1$

(D) $\int \Psi^2 \, d\tau < 0$

6. If an atom or molecule has many electrons, the exact solution of Schrodinger wave equation becomes probably impossible because of :

(A) Many potential energy terms

(B) Many electrons

(C) Electron-electron repulsions

(D) None of these

7. If Ψ is a normalized trial function of an atom or molecule, assigned by the Hamiltonian $\hat{H}$, then according to Varian method the energy of the system may be expressed as :

(A) $\bar{E} = \frac{\int \Psi^* \hat{H} \Psi \, d\tau}{\int \Psi^* \Psi \, d\tau}$

(B) $\bar{E} = \int \Psi^* \hat{H} \Psi \, d\tau$

(C) $\bar{E} = \frac{\int \Psi^* \Psi \, d\tau}{\int \Psi^* \hat{H} \Psi \, d\tau}$

(D) None of these

8. If $\bar{E}$ and E_o are respectively the expected and true values of energy of a quantum mechanical system, then according to variation principle :

(A) $\bar{E} < E_o$

(B) $\bar{E} > E_o$

(C) $\bar{E} - E_o < 0$

(D) None of these

9. If $\hat{H}^o, E^o$ *and* Ψ^o are respectively the Hamiltonian, energy and wave function for the unperturbed state of a system, then perturbation method can be applied only if perturbation is small and :

(A) $\hat{H}^o$ is known

(B) $\hat{H}^o$ and E^o are known

(C) $\hat{H}^o$, E^o and Ψ^o are known

(D) None of these

10. If $\hat{H}^o$ and $\hat{H}$ are the Hamiltonian for the unperturbed and perturbed states of a system and $\lambda\hat{H}'$ is the amount of perturbation, then according to perturbation method :

(A) $\hat{H}^o - \lambda\hat{H}' = \hat{H}$

(B) $\hat{H} = \hat{H}^o + \lambda\hat{H}'$

(C) $\hat{H}^o = \hat{H} + \lambda\hat{H}'$

(D) $\hat{H} = \lambda\hat{H}'$

11. Schrodinger wave equation for H-atom in terms of polar coordinates is :

(A) $\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{\partial^2\Psi}{\partial\phi^2} = 0$

(B) $r^2\frac{\partial\Psi}{\partial r} + \sin\theta\frac{\partial\Psi}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2} = 0$

(C) $\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2} + \frac{8\pi^2 m}{h^2}\left(E + \frac{e^2}{4\pi\epsilon_0 r}\right)\Psi = 0$

(D) None of these

12. To separate the variables of Schrodinger wave equation of H-atom, the wave function Ψ may be expressed as $\Psi(r,\theta,\phi) = R(r)\,T(\theta)\,F(\phi)$

From this equation we can write :

(A) $\frac{\partial\Psi}{\partial r} = T(\theta)\,F(\phi)\frac{\partial R(r)}{\partial r}$

(B) $\frac{\partial\Psi}{\partial r} = R(r)\,F(\phi)\frac{\partial T(\theta)}{\partial r}$

(C) $\frac{\partial\Psi}{\partial r} = R(r)\,T(\theta)\frac{\partial F(\phi)}{\partial r}$

(D) None of these

13. The ϕ-equation is given by :

(A) $\frac{\partial^2 F(\phi)}{\partial \phi^2} = m^2 F(\phi)$

(B) $\frac{\partial^2 F(\phi)}{\partial \phi^2} = \frac{F(\phi)}{m^2}$

(C) $\frac{\partial^2 F(\phi)}{\partial \phi^2} + m^2 F(\phi) = 0$

(D) $\frac{1}{F(\phi)} \frac{\partial^2 F(\phi)}{\partial \phi^2} = m^2$

14. If $m = 0$, the normalized solution of ϕ-equation will be :

(A) $\frac{1}{\sqrt{2}}$

(B) $\frac{1}{\sqrt{2\pi}}$

(C) $\sqrt{2\pi}$

(D) $\frac{\sqrt{2}}{\pi}$

15. For negative values of m, the normalized solutions of ϕ-equation are :

(A) $\frac{1}{\sqrt{\pi}} \cos \phi$

(B) $\frac{1}{\sqrt{\pi}} \sin m \phi$

(C) $\frac{1}{\sqrt{\pi}} \cos m \phi$

(D) $\frac{1}{\sqrt{\pi}} \sin \phi$

16. For $m = +2$, the normalized solution of ϕ-equation will be :

(A) $\frac{1}{\sqrt{\pi}} \cos 2\phi$

(B) $\frac{1}{\sqrt{\pi}} \cos m \phi$

(C) $\frac{1}{\sqrt{\pi}} \sin 2\phi$

(D) $\frac{1}{\sqrt{2\pi}}$

17. The complete wave function of a particle on the surface of a sphere, called spherical Harmonics may be expressed as :

(A) $\underset{l,m}{T(\theta)} \,.\, \underset{n,l}{R(r)}$

(B) $\underset{m}{F(\phi)} \,.\, \underset{n,l}{R(r)}$

(C) $\underset{l,m}{T(\theta)} \,.\, \underset{m}{F(\phi)}$

(D) None of these

18. Spherical harmonics for $l = 0$ and $m = 0$ will be equal to :

(A) $(4\pi)^{1/2}$

(B) $(4\pi)^{-1/2}$

(C) $\frac{1}{\sqrt{2\pi}}$

(D) $(3\pi)^{-1/2}$

19. Spherical harmonics are the wave functions which are orthogonal functions of the polar coordinates :

(A) r and θ

(B) ϕ and r

(C) θ and ϕ

(D) None of these

20. Spin angular momentum or simply 'spin' is given by :

(A) $\sqrt{s(s+1)}$

(B) $\sqrt{s(s+1)}\,\frac{h}{2\pi}$

(C) $\sqrt{s(s+1)}\,\frac{h}{4\pi}$

(D) None of these

21. Spin angular momentum vector, S_z is given by :

(A) $\frac{1}{m_s} \cdot \frac{h}{2\pi}$, where $m_s = \frac{1}{2}$ or $-\frac{1}{2}$

(B) $m_s \frac{h}{2\pi}$, where $m_s = \frac{1}{2}$ or $-\frac{1}{2}$

(C) $m_s \cdot \frac{2\pi}{h}$, where $m_s = \frac{1}{\sqrt{2}}$ or $-\frac{1}{\sqrt{2}}$

(D) $m_s \frac{h}{2\pi}$, where $m_s = -1$ or $+1$

22. If $\alpha(s)$ is the function of a hypothetical spin coordinate, s, then the value of $\nabla^2[\Psi(x, y, z)\alpha(s)]$ will be equal to :

(A) $\nabla^2 \Psi(x, y, z)$

(B) $\alpha(s). \Psi(x, y, z)$

(C) $\alpha(s) \nabla^2 \Psi(x, y, z)$

(D) None of these

23. Electron executes rotational motion around the nucleus in three dimensions, therefore, its position and weve function must be expressed in terms of :

(A) Cartesian coordinates (x, y, z)

(B) Polar coordinates (r, θ, ϕ)

(C) (A) and (B) both

(D) None of these

24. Which of the following factor generally makes the spherical harmonics complex and due to which no real picture can be drawn from them :

(A) $P_l^{|m|} (\cos \theta)$

(B) $e^{im\phi}$

(C) $\sin \theta \cos \theta$

(D) None of these

25. Eigen values of a Hermitian operator are :

(A) Imaginary

(B) Real

(C) λ and λ^*

(D) None of the above

26. Which of the following is the Eigen function for the operator $\frac{d}{dx}$?

(A) $\sin 2x$

(B) e^{ax}

(C) $\sin 3x$

(D) $\cos 2x$

27. The two operators, $\hat{A}$ and $\hat{B}$ are said to be commutative, if :

(A) $\hat{A}.\hat{B}\, f(x) = \hat{B}.\hat{A}\, f(x)$

(B) $\hat{A}.\hat{B}\, f(x) \neq \hat{B}.\hat{A}\, f(x)$

(C) $\hat{A}.\hat{B}\, f(x) = \hat{A}.\hat{A}\, f(x)$

(D) $\hat{A}.\hat{B}\, f(x) = \hat{B}.\hat{B}\, f(x)$

28. The expression for the energy of a particle of mass, m moving in one dimensional box of length, L and infinite hight with potential energy zero inside and infinite outside the box is given by :

(A) $\frac{n^2h^2}{8mL^2}$

(B) $\frac{8mL^2}{n^2h^2}$

(C) $\frac{h^2}{8mL^2}$

(D) $\frac{8mL^2}{h^2}$

29. The normalized wave function for the particle moving in one dimensional box with boundary condition $x = 0$ and $x = L$ can be written as :

(A) $\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}\right) x$

(B) $\sqrt{\frac{L}{2}} \sin\left(\frac{n\pi}{L}\right) x$

(C) $\sqrt{\frac{L}{2}} \sin\left(\frac{L}{n\pi}\right) x$

(D) $\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi Lx}{2}\right)$

30. The energy of a particle in a cubical box having $L_x = L_y = L_z = L$ is given as :

(A) $E = \frac{8m}{h^2}\left(\frac{n_x^2}{L^2} + \frac{n_y^2}{L^2} + \frac{n_z^2}{L^2}\right)$

(B) $E = \frac{h^2}{8mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$

(C) $E = \frac{h^2L^2}{8m}\left(n_x^2 + n_y^2 + n_z^2\right)$

(D) None of the above

31. Total wave function for a particle moving in three dimensional box having sides L_x, L_y and L_z in lengths along X, Y and Z-axes respectively is given by :

(A) $\sqrt{\frac{L_xL_yL_z}{8}} \sin\left(\frac{n_x\pi}{L_x}\right) x \,.\sin\left(\frac{n_y\pi}{L_y}\right) y \sin\left(\frac{n_z\pi}{L_z}\right) z$

(B) $\sqrt{\frac{8}{L_xL_yL_z}} \sin\left(\frac{n_x\pi}{L_x}\right) x \,.\sin\left(\frac{n_y\pi}{L_y}\right) y \,.\sin\left(\frac{n_z\pi}{L_z}\right) z$

(C) $\sqrt{8\, L_xL_yL_z} \sin\left(\frac{n_x\pi}{L_x}\right) x$

(D) None of the above

32. According to Hook law, the restoring force, F is given by the expression :

(A) $F = -k\, x^2$

(B) $F = -k^2$

(C) $F = -k\, x$

(D) $F = -\frac{1}{2}\, k^2\, x$

33. Zero point energy in a simple harmonic motion is equal to :

(A) Zero

(B) $\frac{1}{2} h\, \nu$

(C) $h\, \nu^2$

(D) $h^2\, \nu^2$

34. Vibrational frequency of the linear harmonic oscillator is expressed as :

(A) $\frac{1}{2\pi} \sqrt{k/\mu}$

(B) $\frac{1}{\sqrt{2\pi}} \left(k/\mu\right)^{1/2}$

(C) $\sqrt{2\pi} \sqrt{\mu/k}$

(D) $\sqrt{2}\, k\, \mu$

35. If Ψ_1, Ψ_2 and Ψ_3 are the trial functions of a quantum mechanical system and E_1, E_2 and E_3 respectively are their corresponding expectation values of energy such that $E_2 < E_1 < E_3$. If E_0 is the true energy, then according to variation principle :

(A) E_1 is better approximation to E_0

(B) E_2 is better approximation to E_0

(C) E_3 is better approximation to E_0

(D) None of these

36. If $\phi(i)$ are normalized and mutually orthogonal one-electron wave functions, then the wave function, Ψ of an n-electron atom is assumed to be a simple product of n one-electron wave function i.e. $\Psi = \phi_1(1) \cdot \phi_2(2) \cdot \phi_3(3) \ldots\ldots \phi_n(n)$

This statement is known as :

(A) Fock theory

(B) Hartree's self-consistent field theory

(C) Perturbation theory

(D) Pauli's exclusion principle

37. Hartree-Fock self consistent field theory is based on :

(A) Symmetrized wave function

(B) Antisymmetrized wave function

(C) Eigen function

(D) None of the above

38. The energy of a linear harmonic oscillator in n^{th} energy level is given by :

(A) $\left(n - \frac{1}{2}\right) h\nu$

(B) $\frac{1}{2} h\nu$

(C) $\left(n + \frac{1}{2}\right) h\nu$

(D) None of the above

39. Rotational energy levels for a rigid rotator rotating in three dimensional space are given by the equation :

(A) $E_j = \frac{J(J+1)}{8\pi^2 I}$

(B) $E_j = \frac{8\pi^2 I}{J(J+1)h^2}$

(C) $E_j = \frac{J(J+1)h^2}{8\pi^2 I}$

(D) None of the above

40. Two Eigen function of a Hermitian operator with different Eigen values are mutually :

(A) Orthogonal

(B) Not orthogonal

(C) Symmetric wave functions

(D) None of the above

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