CHE 502
M.Sc.1st SEMESTER EXAMINATION, 2021-22
Chemistry
(Quantum Chemistry-I)
(4+0)
(CBCS Mode)

Important Instruction :	**महत्वपूर्ण निर्देश :**
The question paper is in two sections : Section-A (Descriptive) will be of **15** marks and Section-B (Objective) will be of **60** marks. **Section-A will be deposited at the end of the examination and answer sheet (OMR) of Section-B will be deposited.**	प्रश्न पत्र दो भागो में है : खण्ड–अ (व्याख्यात्मक) **15** अंकों का होगा एवं खण्ड–ब (बहुविकल्पीय) **60** अंक का होगा। **खण्ड–अ परीक्षा के अन्त में जमा कर लिया जायेगा एवं खण्ड–ब का उत्तर पत्रिका (OMR) जमा होगा।**

0234

खण्ड–अ (व्याख्यात्मक)
Section-A (Descriptive)

Time : 1 Hrs.
समय : 1 घण्टे

Max. Marks : 15
अधिकतम अंक : 15

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

अनुक्रमांक (शब्दों में) : _____

Roll No. (In Words) : _____

अभ्यर्थी का नाम : _____

Student Name : _____

कक्ष परिप्रेक्षक के हस्ताक्षर / Invigilator's Signature : _____

Note : (i) Total No. of Questions are Six.
(ii) Answer three questions in all.
(iii) All Questions carry equal marks.

नोट : (i) कुल छः प्रश्न दिए गये हैं।
(ii) किन्हीं तीन प्रश्नों के उत्तर दीजिए।
(iii) सभी प्रश्नों के अंक समान हैं।

1. Discuss the theory of variation method in quantum mechanical calculations with the help of one example.

2. Derive the general expressions for energy levels of a quantum mechanical harmonic oscillator.

3. Discuss the solution of ϕ-equation.

4. What are the postulates of quantum mechanics.

5. Discuss Hartree-Fock self-consistent field theory.

6. Derive the expression for the energy levels of a microscopic particle moving in a three dimensional potential box.

खण्ड–ब (बहुविकल्पीय)
Section-B (Objective)
CHE 502
M.Sc.1st SEMESTER EXAMINATION, 2021-22
Chemistry
(Quantum Chemistry-I)
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AFFIX PRESCRIBED RUBBER STAMP

Date (तिथि) : _____

Paper ID
(To be filled in the OMR Sheet)

0234

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

अनुक्रमांक (शब्दों में) : _____

Roll No. (In Words) : _____

Time : 1½ Hrs.
समय : 1½ घण्टे

Max. Marks : 60
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. The dual nature of matter was predicted by :

(A) Schrodinger

(B) Louis –de- Broglie

(C) G.P. Thomson

(D) Werner Heisenberg

2. The operator $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is called :

(A) Vector operator

(B) Laplacian operator

(C) Hamiltonian operator

(D) Hermitian operator

3. For the operator $\frac{d^2}{dx^2}$, $\sin 2x$ is :

(A) An Eigen function

(B) Not an Eigen function

(C) An Eigen value

(D) None of these

4. It two different acceptable wave functions of a given system are Ψ_i and Ψ_j such that $\int \Psi_i \Psi_j \, d\tau = 0$, then both functions are said to be :

(A) Normalized

(B) Orthogonal

(C) Eigen Values

(D) None of these

5. The operator corresponding to the total energy of a system is called :

(A) Momentum operator

(B) Hamiltonian operator

(C) Laplacian operator

(D) Hermitian operator

6. The energy of a particle of mass m confined to move in one dimensional box f width 'a' and infinite height with potential energy zero inside the box in n^{th} level is :

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

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

(C) $\frac{n^2}{8ma^2}$

(D) $8ma^2$

7. The normalized solution of Schrodinger wave equation for the particle in one dimensional box is :

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

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

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

(D) $\sin\left(\frac{n\pi x}{a}\right)$

8. In the case of a particle in one dimensional box, the Eigen functions are :

(A) Orthogonal

(B) Not Orthogonal

(C) (A) and (B) both

(D) None

9. The total energy, E of a particle moving in a three dimensional rectangular box having sides a, b, and c in lengths along x, y and z – axes respectively is :

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

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

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

(D) None of these

10. The square of the magnitude of the wave function is called :

(A) Current density

(B) Probability density

(C) Zero density

(D) Volume density

11. The vibrational energy of a simple harmonic oscillator for vibrational quantum no. 3 will be :

(A) $2\,h\nu$

(B) $4\,h\nu$

(C) $\frac{7}{2}\,h\nu$

(D) $\frac{5}{2}\,h\nu$

12. Any Wave function can be written as a linear combination of :

(A) Eigen Vectors

(B) Eigen Values

(C) Eigen functions

(D) Operators

13. According to variation method, is Ψ is a trial function of a quantum mechanical system, described by the Hamiltonian $\hat{H}$, then the energy of the system is approximately given by :

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

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

(C) $\overline{E} = \int \Psi^* \Psi d\tau$

(D) None of these

14. According to variation principle, the expectation value of energy, $\overline{E}$ will always be:

(A) Greater than the true energy, E_0

(B) Less than the true energy, E_0

(C) Zero

(D) None of these

15. Perturbation method can be used only if :

(A) The perturbation is large

(B) The perturbation is small

(C) The perturbation is zero

(D) None of these

16. If $\hat{H}^0$ is the Hamiltonian in the unperturbed state, $\hat{H}$ that of the perturbed state and $\lambda\hat{H}'$ is the amount of perturbation, then the perturbed Hamiltonian is given by :

(A) $\hat{H} = \hat{H}^0 + \lambda\hat{H}'$

(B) $\hat{H}^0 = \hat{H} + \lambda\hat{H}'$

(C) $\hat{H}^0 - \lambda H' = \hat{H}$

(D) None of these

17. Frequency of the linear harmonic Oscillator is :

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

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

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

(D) $2\pi k$

18. Which is not the condition for acceptable wave function ?

(A) Continuous

(B) Finite

(C) Linear

(D) Single valued

19. If Ψ_1 and Ψ_2 are the Eigen functions of the operator $\hat{A}$ such that $\int \Psi_1^* (\hat{A}\Psi_2) d\tau = \int (\hat{A}\Psi_1)^* \Psi_2 d\tau$, then the operator $\hat{A}$ is said to be :

(A) Hermitian operator

(B) Hamiltonian operator

(C) Laplacian operator

(D) None of these

20. In terms of Laplacian operator, the Schrodinger wave equation can be written as:

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

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

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

(D) None of the above

21. A Hermitian operator has :

(A) Real Eigen values

(B) Imaginary Eigen values

(C) (A) and (B) both

(D) None of these

22. Two operators $\hat{A}$ *and* $\hat{B}$ are said to be commute, if :

(A) $\hat{A}\hat{B} = \hat{B}\hat{A}$

(B) $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

(C) $\hat{A}\hat{B} + \hat{B}\hat{A} = 0$

(D) None of above

23. The wave function, Ψ of an n- electron atom is assumed to be a simple product of n one-electron wave functions $i - e' \Psi = \phi_1(1)\phi_2(2)\phi_3(3) \ldots\ldots \phi_n(n)$; where $\phi(i)$ are normalized and mutually orthogonal one electron wave functions. This is the statement of :

(A) Hartree self-consistent field theory

(B) Variation theory

(C) Perturbation theory

(D) Pauli exclusion principle

24. In quantum mechanics, the uncertainty principle is given by :

(A) Plank

(B) De Broglie

(C) Schrodinger

(D) Heisenberg

25. Quantum mechanics is applicable for :

(A) Microscopic objects

(B) Macroscopic objects

(C) (A) and (B) both

(D) None of these

26. The probability of finding the electron at particular point is given by :

(A) Ψ^2

(B) Ψ

(C) $\frac{\Psi}{2}$

(D) 2Ψ

27. For positive values of m, the normalized solutions of ϕ − equation are :

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

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

(C) $\frac{1}{\sqrt{3\pi}}$

(D) None of these

28. For the separation of variables of Schrodinger wave equation of H atom, the wave function Ψ may be expressed as :

(A) $\Psi = \frac{R(\gamma)T(\theta)}{F(\phi)}$

(B) $\Psi = R(\gamma)T(\theta)F(\phi)$

(C) $\Psi = \frac{F(\phi)}{R(\gamma)T(\theta)}$

(D) $\Psi = R(\gamma)T(\theta) - F(\phi)$

29. $\frac{a}{\sqrt{\pi}} Sin\, m\emptyset$ are the normalized solutions of $\emptyset$ – equation for :

(A) Negative values of m

(B) Positive values of m

(C) $m = 0$

(D) None of these

30. The de Broglie relation is :

(A) $\lambda = \frac{h}{mv}$

(B) $E = mc^2$

(C) $\lambda = \frac{h}{2\pi}$

(D) $\lambda = \frac{h}{mv^2}$

31. Which of the following is the normalized solution of ϕ – equation for $m = 0$:

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

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

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

(D) 2π

32. The radial distribution of the electron is described by the function :

(A) $R(\gamma)$

(B) $T(\theta)$

(C) $F(\phi)$

(D) None of these

33. Which of the following are called angular wave functions :

(A) $R(\gamma)$ and $T(\theta)$

(B) $R(\gamma)$ and $F(\phi)$

(C) $T(\theta)$ and $F(\phi)$

(D) None of these

34. The correct form of Schrodinger wave equation is :

(A) $\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h} E\Psi = 0$

(B) $\frac{d^2\Psi}{dx^2} + \frac{h^2}{8\pi m} E\Psi = 0$

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

(D) $\frac{d^2\Psi}{dx^2} + \frac{d^2\Psi}{dy^2} + \frac{d^2\Psi}{dz^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$

35. Which of the following is called radial wave function :

(A) $R(\gamma)$

(B) $T(\theta)$

(C) $F(\emptyset)$

(D) (B) and (C) both

36. The wave functions, $Y_{l,m}(\theta, \emptyset) = T_{l,m}(\theta)F_m(\emptyset)$ are called :

(A) Spherical harmonics

(B) Radial wave functions

(C) (A) and (B) both

(D) None of these

37. The $\theta -$ equation is given by :

(A) $\frac{\sin\theta}{T(\theta)} = m^2$

(B) $\frac{\sin\theta}{T(\theta)}\frac{\partial}{\partial\theta}\left[\sin\theta\ \frac{\partial T(\theta)}{\partial\theta}\right] + \beta\sin^2\theta = m^2$

(C) $\beta\sin^2\theta = m^2\ T(\theta)$

(D) None of these

38. The velocity of a particle moving with simple harmonic motion at the mean position is :

(A) Zero

(B) Minimum

(C) Maximum

(D) One

39. The radial wave function gives :

(A) The size of orbitals

(B) The shape of orbitals

(C) The shape and size of orbitals

(D) None of these

40. In an acceptable wave function, Ψ of a given system is such that $\int \Psi^2 d\tau = 1$, then the wave function, Ψ is said to be :

(A) Normalized

(B) Orthogonal

(C) Orthonormal

(D) None of these

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