[92] SEAT No._____ No. of Printed Pages : 2

SARDAR PATEL UNIVERSITY

M.Sc. (SEMESTER-II) EXAMINATION

Monday, 22nd October, 2018

Time: 10:00 a.m. to 01:00 p.m.

CHEMISTRY: PS02CCHE21

(QUANTUM CHEMISTRY)

Time: - 3 hours **Marks:-70**

[h = 6.626 x 10^{-34} J.S., 1J = 6.24 x 10^{18} eV, 1a.u. = 0.435 x 10^{-17} J]

Que-1. Answer the following. **[8]**

1. The value of $(\partial/\partial x)\ \psi$ = _____.
   (a) ψ (b) $-\psi$ (c) 0 (d) None of them
2. Which of the following indicates non-degenerate state?
   (a) E_{112} (b) E_{111} (c) E_{221} (d) E_{121}
3. In case of spring, Hooke's low is represented by the equation:
   (a) K = Xf (b) K = - Xf (c) F = - kx (d) F = kx
4. In transforming Cartesian coordinates into polar coordinates, Z = _____.
   (a) $r\sin\theta\cos\phi$ (b) $r\cos\theta$ (c) $r\sin\theta$ (d) $r\sin\theta\sin\phi$
5. For large value of n, _____ behaves like a Taylor series of expansion.
   (a) Recursion series (b) Laguerre Series
   (c) Power series (d) None of them
6. What is the nature of O_2 according to VBT?
   (a) Paramagnetic (b) Diamagnetic (c) Both a & b (d) Antiferromagnetic
7. α is spin Eigen function corresponding to λ = _____.
   (a) +1/2 (b) -1/2 (c) +1/4 (d) -1/4
8. The symbol corresponds to Laplacian operator is_____.
   (a) ∇ (b) ∇^2 (c) L (d) L^2

Que-2. Answer the following. [Any seven] **[14]**

(1) Explain the Schmidt orthogonalization process.
(2) What are the applications of Quantum mechanical tunneling?
(3) Show that $\hat{P}y = h/2\pi\ i \times \partial/\partial y$.
(4) Derive the equation $T = L^2/2I$.
(5) Determine L, S, J & term symbol arising out of coupling between an electron in p-orbital and another in d-orbital.
(6) Find out the radial Eigen function for 1S system.
(7) Derive the first order perturbation energy equation.
(8) Give the complete wave function of N_2 & O_2 molecules.
(9) Explain the bonding in HeH molecule on the basis of valence bond treatment.

(1) (P.T.O.)

Que-3. **[A]** Explain the Quantum mechanical tunneling in detail. **[6]**

[B] Explain the translational motion of free particle system. **[6]**

OR

[B] Answer the following. **[6]**

(i) Show that (Lx, Ly) is non commute and (L^2, Lx) is commute.

(ii) What is Quantization? Calculate energy gap for:

(a) An electron in a box of length 10 A°. (b) A particle of mass 0.1 gm in a box of length 10 cm. Comment on quantization for both the cases.

Que-4. **[A]** Derive the Radial equation for large & small value of ρ. **[6]**

[B] Diatomic molecule CO rotates in free axis and fixed axis. Calculate first four energy levels and angular momentum. Also calculate absorption frequency and wavelength of light absorbed when transition take place from ground state to first excited state. Intermolecular distance in CO is 1.2×10^{-10} m. **[6]**

OR

[B] Answer the following.

(i) Derive the Schrodinger equation and energy equation for the vibrational motion of particle in one dimensional harmonic oscillator. **[4]**

(ii) Derive the forth degree of hermite's polynomial. **[2]**

Que-5. **[A]** Define Dirac notation. Explain the time - independent perturbation theory for non degenerate state. **[6]**

[B] Derive the normalized wave function for many electron system. **[6]**

OR

[B] Answer the following. **[6]**

(i) Derive the equation $\bar{E} = a_1^2 E_1 + a_2^2 E_2$.

(ii) Prove that repulsion energy term is important, when we calculating total energy and ionization energy of helium atom. Experimental values are -78.4 eV& 24.6 eV for calculating total energy and ionization energy respectively. Here J = 1.25 a.u.

Que. 6. **[A]** Derive the electronic and nuclear Schrodinger equation using Born Oppenheimer approximation. **[6]**

[B] Derive the term symbol for the following. **[6]**

(i) H_2^+ (ii) N_2 (iii) O_2 (iv) H_2 (Excited)

OR

[B] Explain the molecular orbital theory for hydrogen molecule ion. **[6]**

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