(33 & A-9) Seat No: _____ No. of Printed Pages : 3

SARDAR PATEL UNIVERSITY

M.Sc. (SEMESTER-I) EXAMINATION
Friday, 21st Oct., 2016
10:00 A.M. to 01:00 P.M.
CHEMISTRY: PS01CCHE01
(INORGANIC CHEMISTRY-I)

Note:-figures to the right indicate full marks: **Total marks: 70**

Que : 1 Answer the following: **[8]**

1. Normalization wave function for rotational motion of a particle in ring is _____.
   (a) $1/\sqrt{2\pi}\exp(\pm im\Phi)$ (b) $1/\sqrt{4\pi}\exp(\pm im\Phi)$
   (c) $1/4\pi\exp(\pm im\Phi)$ (d) $1/2\pi\exp(\pm im\Phi)$
2. The symbol corresponds to Laplacian operator is
   (a) ∇^2 (b) ∇ (c) L (d) $\hat{L}$
3. The solution of radical equation fpr small value of ρ is.....
   (a) $\frac{R}{4}$ (b) $\frac{4}{R}$ (c) $\frac{2}{R}$ (d) $\frac{R}{2}$
4. Perturbation method is applied to the system is.....
   (a) $\hat{H}^0 >>> \hat{V}$ (b) $\hat{V} >>> \hat{H}^0$ (c) $\hat{H}^0 = \hat{V}$ (d) None of these
5. The value of associated languerre polynomial for n=3 and l=2 system is.....
   (a) 120 (b) -120 (c) 6 (d) -6
6. What will be the effect on the bond strength, if H-atom in C-H bond is replace by T to form C-T bond?
   (a) Bond strength increase (b) bond strength remain same
   (c) bond strength decrease (d) bond cannot form
7. The term symbols for B_2 molecule is:
   (a) $^3\Sigma_g$ (b) $^3\Pi_u$ (c) $^2\Sigma_g$ (d) $^3\Sigma_u$
8. A system represented by function $\Psi = \sqrt{\frac{1}{8}}\Phi_1 + \sqrt{\frac{7}{8}}\Phi_2$ the probability of getting the value of energy E_1 is....
   (a) $\frac{1}{8}$ (b) $\sqrt{\frac{7}{8}}$ (c) $\sqrt{\frac{1}{8}}$ (d) $\frac{7}{8}$

Que : 2 Attempt any SEVEN of the following: **[14]**

1. Evaluate the commutator [Y, d/dz].
2. Explain the total wave function for hydrogen like atom.
3. Calculate the energy of the state E_{121} by distortion along Y-axis and show the effect of distortion on the energy
4. Derive second order perturbation energy equation.
5. State the average kinetic energy is equal to E, $\Psi = \sin kx$.
6. The $\pi_u 2Px$ orbital is lower in energy than $\sigma_g 2Pz$ for the C_2 system, Explain
7. Explain position, momentum and uncertainty relation.
8. Derive the Schrödinger's equation for particle in one dimensional harmonic oscillator.
9. Explain the bonding in HF on the basis of VB treatment.

(P.T.O.)

Que: 3 (A) Butadiene contains 4π electron each of which moves freely from one end of the molecule to the other. Treat the molecule as a one dimensional box whose box length is equal to the length of carbon chain plus half C-C bond length on either other sides. The average C-C bond length is 0.14 nm. [6]

(i) Calculate the total ground state energy of the molecule.

(ii) Calculate the lowest absorption frequency(in cm^{-1}) and wave length(in nm) of light absorbed.

(Given : h= 6.626×10^{-34} JS, 1J = 6.24×10^{18} and 1eV = 8.06×10^{3} eV cm^{-1})

Que: 3 [B] **Answer the following:**

(I) Show that set-down operator does not commute with set-up operator but commute with square of angular momentum operator. [3]

(II) Discuss the translational motion of the particle in a cubical box. [3]

OR

Que: 3 [B] Write a note on quantum mechanical tunneling and write its two applications. [6]

Que: 4[A] Assuming harmonic oscillator model for C-C, C=C, C≡C bond having frequency 1400, 1700 and 2100 cm^{-1} respectively. [6]

(i) Calculate the bond strength. (force constant)

(ii) Calculate the lowest vibration energy level.

(iii)Calculate the energy gap between two levels.

Que: 4 [B] **Answer the following:**

(I) Derive the Recursion formula for Hermite's differential equation for one dimensional harmonic oscillator. [3]

(II) Derive the associated languerre polynomial for n=3 and l=2. [3]

OR

Que: 4 [B] Considering CO as a rigid rotator in a (I) XY-plane (II) three dimension. [6]

(I) Calculate the frequency and wave length of light emitted when transition takes place from exited stage to ground state, i.e. n=1 to n=0

(II) Calculate the angular momentum and first three rotational energy level.

[Given: Radius=1×10^{-10} m, h= 6.626×10^{-34} JS, C= 3×10^{8} m/sec]

Que :5 [A] Derive the normalized wave function. [6]

$\Psi_{(1,2,3,\ldots,n)} = 1/\sqrt{n!}\ |\Phi_1(1), \Phi_1(2), \ldots\ldots \Phi_{n/2}(n)|$ for many electron systems.

Que: 5 [B] Answer the following:

(I) Derive the time-independent perturbation theory for non degenerate state and calculate the first order perturbation energy equation. **[3]**

(II) Explain: Hartree's self consistent field method. **[3]**

OR

Que: 5 [B] Answer the following:

(I) Using the function $Y = \rho^k . e^{-\rho}$ Derive the radial normalized wave function for one electron system. **[3]**

(II) Calculate the total energy and ionization energy of the He atom in presence and absence of repulsion energy and compare with experimental value. **[3]**

[1 a.u.= 0.435×10^{-17} JS, and 1J= 6.24×10^{18} eV]

Que: 6 [A] Derive the energy equation $H_{AA} = 2E_H + 1/R + J$ for hydrogen molecule on the basis of Heitler and London theory. **[6]**

[B] Answer the following:

(I) Discuss the adiabatic and crude Born Oppenheimer approximation. **[3]**

(II) Explain LCAOMO treatment for diatomic molecule. **[3]**

OR

Que: 6 [B] Answer the following:

(I) Explain the electronic state and term symbols for diatomic molecule. Determine the term symbols for He_2^+, O_2, F_2^+. **[3]**

(II) Discuss the angular momentum for many electron systems. **[3]**

All the best

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