[50]

SARDAR PATEL UNIVERSITY
M.Sc. (Chemistry) (First Semester)(CBCS)EXAMINATION
2012
Friday, 30th November
PS01CCHE- 01 (Inorganic Chemistry-I)

Time: 10.30 am to 1.30pm   Total marks:-70

Q-1. Answer the following: **(8)**

1. If $\hat{A} = d/dx$, $\hat{B} = d^2/dx^2$ and $f(x) = \sin x$ then what is the relation between $\hat{A}\hat{B}f(x)$ and $\hat{B}\hat{A}f(x)$.
    (a) Equal   (b) Less   (c) greater   (d) Not equal

2. The lowest energy in a cubical box is given by the equation:
    (a) $E = h^2/8mL^2$ (b) $E = 6h^2/8mL^2$ (c) $E = 3h^2/8mL^2$ (d) $E = 2h^2/8mL^2$

3. At the extreme point ($\pm a$) of oscillation, all the energy is:
    (a) Electrical   (b) Potential   (c) Kinetic   (d) Nuclear

4. H-like systems are characterized by _____ .
    (a) $V = -Z^2e^2/(4\pi\varepsilon_0)r$ (b) $V = +Ze^2/(4\pi\varepsilon_0)r$
    (c) $V = +Z^2e^2/(4\pi\varepsilon_0)r$ (d) $V = -Ze^2/(4\pi\varepsilon_0)r$

5. A simple harmonic oscillator is an _____ system?
    (a) perturbed   (b) None   (c) unperturbed   (d) both a & b

6. The "Spin-multiplicity" corresponding to S=2 is:
    (a) quintuplet   (b) quadruplet   (c) doublet   (d) singlet

7. The energy required by H_2^+ for dissociation is:
    (a) 1.60 eV   (b) 1.06 eV   (c) 2.97 eV   (d) 2.79 eV

8. What is the nature of O_2 according to VBT?
    (a) Paramagnetic   (b) Diamagnetic   (c) both   (d) none of them

Q-2. Answer the following: [Any seven]   **(14)**

1. Show that: Average kinetic energy of electron in a one dimensional box is equal to $n^2h^2/8mL^2$.
2. Determine the value of associated Laguerre polynomial for $n = 3$ & $l = 2$.
3. Find out the third degree of polynomial.
4. Show that $[AB,C] = \hat{A}(B, C) + (\hat{A}, C)B$.
5. Derive second order perturbation energy equation.
6. A closed shell electronic configuration always gives rise to the term ^1S; explain why?
7. Calculate the energy of state E_{122} by distortion along Y-axis and show the effect of distortion on energy.
8. Explain the ionic contribution for hydrogen molecule on the basis of VBT.
9. What are the conditions for atomic orbital's to undergo linear combination.

Q-3. Answer the following: **(6)**

(A) Butadiene contains 4 π e- each of which moves freely from one end of the molecule to another end. Treat the molecule as one dimensional box whose length is equal to sum of all C-C bond length plus half the C-C bond length on either side. The average C-C bond length is 0.14nm.
1. Calculate the lowest absorption frequency in cm^{-1} and wave length (λ) in nm of light absorbed.
2. Calculate the total ground state energy.
    [Given: $h = 6.626 \times 10^{-34}$ JS, $1J = 6.24 \times 10^{18}$ eV, $1eV = 8.06 \times 10^3$ cm^{-1}]

(B)   Write a note on: Quantum Mechanical tunneling and write its application.   (6)

Or

(B)   **Answer the following:**
  1. Show that the raising and lowering operators neither commute with component of angular momentum operator nor with each other but commute with square of angular momentum operator.
  2. Write the utility of box model with suitable example.

Q-4.   Answer the following: (6)
(A)   Considering NO as a rigid rotator rotates in: (i) XY- plane & (ii) Three dimension.
  1. Calculate 1st three rotational energy level & Angular momentum.
  2. Calculate wavelength & frequency of radiation emitted when transition takes place from excited state to ground state ($n=3 \rightarrow 2 \rightarrow 1$) level. [Given: $r = 1.15 \times 10^{-10}$].
(B)   Derive the Schrodinger equation & Hermite's differential equation for vibrational motion of a particle in a one dimensional harmonic oscillator.   (6)

Or

(B)   **Answer the following:**
  1. Explain: Normalization of wave function for a rotational motion of a particle in a ring.
  2. Explain: Total wave function for H-like atom.

Q-5.   Answer the following: (6)
(A):1. Explain: Hartree's self consistent field method.
  2. A system is represented by function $\Psi = \sqrt{5}/\sqrt{9}\ \Phi_1 + \sqrt{4}/\sqrt{9}\ \Phi_2$. Where Φ_1 & Φ_2 are orthonormal function. What will be the probability of getting the energies E_1 & E_2 as an eigen value of Φ_1 & Φ_2 respectively?
(B):   **Answer the following:**
  1. Derive the wave function for many $-e^-$ system.   (6)
  2. Explain: Commutation with Hamiltonian.

Or

(B):   **Answer the following:**
  1. Derive the first order correction to the wave function of the time independent. **(3)** Perturbation theory for non-degenerate state
  2. Explain spin-multiplicity, term-multiplicity and levels with suitable examples. **(3)**

Q-6.   Answer the following: (6)
(A):   Derive the energy equation $E = 2E_H + 1/_R + J - 2\ (J + k\ /\ 1 + s)$ for H_2 molecule on the basis of molecular orbital theory and show that error in calculated value of energy is about 56% compared to experimental value.
(B):   **Answer the following:**   (6)
  1. Explain the bonding in HeH on the basis of VB treatment and ionic contribution in HF.
  2. Explain: The electron density distribution in symmetric and asymmetric states in Heitler and London theory.

Or

(B):   Derive the energy equation $H_{AA} = 2E_H + 1/R - J$ for hydrogen molecule on the basis of Heiter-London theory.

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