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SARDAR PATEL UNIVERSITY

M.Sc. (SEMESTER-I) EXAMINATION

Tuesday, 19th March, 2019
Time: 10:00 a.m. to 01:00 p.m.
CHEMISTRY: PS01CCHE01
(Inorganic Chemistry-I)

Time: - 3 hours Marks:- 70

Que. 1. Answer the following. [8]

1. At the equilibrium point (x=0) of oscillation all the energy corresponds to_____.
   (a) Potential energy (b) Rotational Energy
   (c) Kinetic Energy (d) Electronic Energy
2. The _____is zero-point energy for harmonic oscillator.
   (a) 1/2 hν (b) 3/2 hν (c) hν (d) 5/2 hν
3. _____ is the number of term for $L \geq S$
   (a) $2S + 1$ (b) $2L + 1$ (c) $2(L + 1)$ (d) $2(S + 1)$
4. The average kinetic energy of free particle is _____
   (a) $n^2h^2/8ML^2$ (b) $k^2h^2/8M\pi^2$ (c) $n^2h^2/8M\pi^2$ (d) $k^2h^2/8ML^2$
5. Perturbation method is applied to the system _____
   (a) For the unperturb state E^0 not known & Ψ^0 known.
   (b) For the unperturb state E^0 & & Ψ^0 known.
   (c) For the unperturb state E^0 known & Ψ^0 not known.
   (d) For the unperturb state E^0 & Ψ^0 are not known.
6. _____ is the value of associated Laguerre polynomials for 1s orbital.
   (a) 6 (b) 1 (c) -6 (d) -1
7. The energy required for dissociation by H_2^+_____H_2
   (a) > (b) < (c) ≥ (d) ≤
8. The value of spin multiplicity for C_2^+ molecule is:
   (a) 4 (b) 1 (c) 2 (d) 3

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

(1) Define the term: (i) Zero point energy (ii) Constant of motion
(2) Explain the commutative property giving suitable examples.
(3) Write a note on Hamiltonian operator.
(4) Explain the total wave function for hydrogen like atom.
(5) Determine the value of associated Laguerre polynomial for n=3 and l=0 system.
(6) Give the condition for perturbation treatment.
(7) Define the term: Dirac notation and Perturbation.
(8) Explain the σ and π-molecular orbitals.
(9) Explain the bonding in LiH molecule.

(P.T.O.)

Que. 3. [A] Butadiene contains 4π ē 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 0.14 nm. [6]

(i) Calculate the lowest absorption frequency (υ) in cm^{-1} & wave length (λ) in nm of light absorbed.

(ii) Calculate the total ground state energy.

(Given: $h=6.26 \times 10^{-34}$ Js, $1J = 6.24 \times 10^{18}$ eV and $1\ eV = 8.06 \times 10^{3}\ cm^{-1}$)

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

OR

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

1. Explain square of angular momentum and its component (X,Y) Commute with each other.
2. Discuss the translational motion of a cubical box.

Que. 4. [A] Derive Hermit's differential equation and Recursion formula. [6]

[B] Assuming harmonic oscillator model for C-C, C=C and C≡C with frequency $1400cm^{-1}$, $1700cm^{-1}$ and $2100cm^{-1}$ respectively. Calculate bond strength, lowest vibrational energy and energy gap between two levels. [6]

OR

[B] Derive the radical function for small, large and intermediate value of ρ. [6]

Que. 5. [A] Derive the time - independent perturbation theory for non degenerate state and calculate the second order perturbation energy equation. [6]

[B] Explain the spin-orbit interaction. Derive the term symbols arising out of coupling between an electron in d-orbital and f-orbital. [6]

OR

[B] (i) Explain the commutation with Hamiltonian [3]

(ii) Explain variation method. [3]

Que. 6. [A] Explain the LCAO-MO treatment of diatomic molecule and differentiate the π-MO's and σ-MO's. [6]

[B] Discuss the Born- Oppenheimer approximation for the solution of Schrodinger equation. [6]

OR

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

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