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SARDAR PATEL UNIVERSITY
M.Sc. (SEMESTER-I) EXAMINATION
Monday, 18th November,2019
Time: 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**

Q.1.Answer the following: **[8]**

1. The _____is zero-point energy for harmonic oscillator.
   a) 1/2 hν b) 3/2 hν c) hν d) 5/2 hν
2. _____ operator has not zero value.
   a) (d,d/dx)Ψ b) (x,d/dy) Ψ c) (d/dx,d^2/dx^2) Ψ d) (d/dy,x)Ψ
3. The solution of radical equation for small value of ρ is _____
   a) $\frac{R}{2}$ b) $\frac{4}{R}$ c) ρ^l d) $\frac{R}{4}$
4. Perturbation method is applied to the system is _____
   a) None of these b) $\hat{V} >>> \hat{H}^0$ c) $\hat{H}^0 = \hat{V}$ d) $\hat{H}^0 >>> \hat{V}$
5. The value of associated Laguerre polynomial for n=3 and l=2 system is ___
   a) 120 b) -120 c) 6 d) -6
6. At the equilibrium point (x=0) of oscillation all the energy corresponds to_____
   (a) Rotational Energy (b) Kinetic Energy
   (c) Potential energy (d) Electronic Energy
7. The term symbols for B_2 molecule is:
   (a) $^2\Sigma_g$ (b) $^3\Pi_u$ (c) $^3\Sigma_g$ (d) $^3\Sigma_u$
8. The operator corresponds to total energy of the system is_____
   (a) P (b) $\hat{Z}$ (c) $\hat{H}$ (d) ALL

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

1. Write a note on Hamiltonian operator.
2. Calculate the energy of state E_{121} by distortion along Y-axis and show the effect of distortion on energy.
3. Explain the commutative property giving suitable examples.
4. Derive first order perturbation energy equation.
5. Derive the Laguerre polynomial for n=3 & l=1
6. State the average kinetic energy is equal to E, Ψ = sin kx.
7. What is Dirac notation?
8. Derive the term symbol for N_2^+.
9. Determine the Value of L, S, J and the term symbol arising out of the coupling between an electron in s – orbital and an electron in p – orbital.

Q.3.A. Write a note quantum mechanical tunneling and write its two applications. **[06]**

Q.3.B. Answer the following: **[06]**

1. Give the list of first two symmetric and asymmetric wave function along with eigenvalue for a particle in a box. Find out the values of normalized wave function at X = 0, ± L/2 and ± L/4 for first symmetric and asymmetric wave function.
2. Show that [Lx, Ly] ≠ 0.

OR

B. Butadiene contain $4\pi e$, each of which moves freely from one end of the molecules to the other. Treat the molecules as a one dimensional box whose length is equal to the length of C-C bond plus half of the C-C bond length on either side. The average C-C bond length is 0.14 nm. **[06]**

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

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

(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})

Q.4.A. Answer the following: **[06]**

1. Derive the third degree of Hermit's polynomial.

2. Explain rotation of a diatomic molecule in a plane.

B. Assuming harmonic oscillator model for C-C, C=C and C≡C with frequency. **[06]** 1450cm^{-1}, 1750cm^{-1}, 2100cm^{-1} respectively. Calculate bond strength, lowest vibrational energy and energy gap between two levels.

OR

B. Answer the following: **[06]**

1. Derive the normalization factor of the wave function for a one dimensional.

2. Derive the radial function for large & small value of ρ.

Q.5.A. Derive the time independent perturbation theory for non-degenerate state and calculate first order perturbation energy equations. **[06]**

B. Discuss the wave function for the many electron systems. **[06]**

OR

B. Answer the following: **[06]**

1. Explain the commutation with the Hamiltonian.

2. Explain: Hartree's self-consistent field method.

Q.6.A. Derive the energy equation $H_{AA} = 2E_H + \frac{1}{R} + J$ for Hydrogen molecule on the basis of Heitler & London theory. **[06]**

B. Answer the following: **[06]**

1. Discuss the Born-Oppenheimer approximation for the solution of Schrodinger equation.

OR

B. Answer the following: **[06]**

1. Determine the term Symbols for He_2^+, O_2, F_2^+.

2. Explain LCAOMO treatment for diatomic molecule.

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