SEAT No._____ No. of Printed Pages : 2

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SARDAR PATEL UNIVERSITY

M.Sc. (SEMESTER-I) EXAMINATION
Monday, 9th April, 2018
Time: 10:00 a.m. to 1:00 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 symbol corresponds to Laplacian operator is _____.
   (a) ∇^2 (b) ∇ (c) L (d) L^2

2. The term symbol for L= 3 and S=0 system is _____.
   (a) $^1D_3$ (b) $^1F_3$ (c) $^3F_2$ (d) $^3D_2$

3. When electrons are free in atoms and molecules they undergo _____ motion?
   (a) Rotational (b) Vibrational (c) Linear (d) None of them

4. Which of the following indicates non degenerate state?
   (a) E_{112} (b) E_{121} (c) E_{221} (d) E_{222}

5. At the extreme point (±a) of oscillation, all the energy is:
   (a) Potential (b) Electrical (c) Kinetic (d) Nuclear

6. Born Openheimer approximation is very reliable for _____ electronic state.
   (a) Excited (b) Ground (c) both a & b (d) None

7. In vibrational motion of particle, as **n** increase the energy gap also_____.
   (a) Increase (b) decrease (c) Constant (d) none of these

8. In H_2^+ ion the bond distance and bond dissociation energy is_____&_____.
   (a) 1.79Å, 2.06 eV (b) 1. 06 Å, 2.79 eV (c) 1. 06 Å, 2.69 eV (d) 1.60 Å, 2.97 eV

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

1. Derive the Schrodinger equation for particle in one dimensional oscillator.
2. Write a note on Hamiltonian operator.
3. Define the term (i) Zero Point Energy (ii) constant of motion
4. Show that : $\hat{P}_X = \frac{\pm h}{2\pi i}\frac{d}{dx}$
5. Explain the total wave function for hydrogen like atom.
6. Explain the bonding in HF on the valance bond theory.
7. Derive the Laguerre polynomial for n=3 & l = 2.
8. Determine L, S, J & term symbol arising out of coupling between an electrons in p-orbital & another in d-orbital.
9. Explain the ionic contribution for hydrogen molecule on the basis of VBT.

C.P.T.O.

Q.3.A. Write a note on quantum mechanical tunneling and write its two uses. **[6]**

B. 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= 6.626×10^{-34} JS, 1J= 6.24×10^{18} eV, and 1eV= 8.06×10^{3} cm^{-1}]

OR

B. Answer the following.

(i) Explain square of angular momentum and its component (X, Y) Commute with each other. **[3]**

(ii) Discuss the translational motion of a cubical box. **[3]**

Q.4.A. Derive Hermite's differential equation and Recursion formula. **[6]**

B. 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

(ii) Calculate the lowest vibrational energy

(iii) Calculate the energy band gap between two energy level

OR

B. (i) Explain rotational motion of diatomic molecule can occur in a plane. **[3]**

(ii) Derive radial eigen function for n=1 and l=0 system. **[3]**

Q.5.A. Explain wave function for many electron system. **[6]**

B. Explain time independent theory for non-degenerate system. Also find out first and second order perturbation energy equation. **[6]**

OR

B. Answer the following.

(i) Discuss the commutation with Hamiltonian. **[3]**

(ii) Explain Hatree self consistent field method. **[3]**

Q.6.A. Explain Born Oppenheimer approximation for the solution of Schrodinger equation. **[6]**

B. Explain the LCAO-MO treatment of diatomic molecule and differentiate the π-MO's and σ – MO's. **[6]**

OR

B. Derive the equation $E = 2E_H + \frac{1}{R} + J - 2\frac{(J+k)}{(1+S)}$ for hydrogen molecule on the basis of MOT. **[6]**