[70] SEAT No._____ No of printed page: 3

SARDAR PATEL UNIVERSITY

M.Sc. (SEMESTER-I) EXAMINATION
Tuesday, 23rd October, 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 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) $k^2h^2/8ML^2$

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

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

4. Perturbation method is applied to the system if:
   (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.

5. H- like atom are characterized by :
   (a) $+Ze^2/(4\pi E_0)r$ (b) $-Ze^2/(4\pi E_0)r$ (c) $+ \frac{1}{2} Ka^2$ (d) $- \frac{1}{2} Ka^2$

6. What is the nature of O_2 according to VBT ?
   (a) Paramagnetic (b) Diamagnetic
   (c) Both a & b (d) Antiferromagnetic

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

(P.T.O.)

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

1. Write a note on Hamiltonian operator
2. Prove $[Ly, Lz] = i\hbar\hat{L}x$
3. Derive the n^{th} order perturbation energy equation.
4. Determine L, S, J & term symbol arising out of coupling between an electron in p-orbital & another in d-orbital.
5. For a particle in a box, explain how the particle quantization of energy depends on the size of the box, size of the particle and wavelength of the light.
6. Determine the value of associated Laguerre polynomial for n=3 and l=2 system.
7. Derive the Hermite's polynomial for third degree.
8. Explain electro density and bonding in H_2^+ ion on basic of MOT.
9. Show that component of angular momentum operator Lz does not commute with set down operator.

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

B. Answer the following.

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

(ii) Explain: Normalization of wave function for a rotational motion of a particle in a ring **[3]**

OR

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: $h= 6.626\times10^{-34}$JS, $1J=6.24\times10^{18}$ eV, and $1eV= 8.06\times10^{3}$ cm^{-1}]

Q.4.A. Derive the radial function for large, small and intermediate value of ρ. **[6]**

Q. 4. B. Considering Hydroiodic (HI) acid as a rigid rotator rotating in **[6]**

(i) XY plane (ii) Three dimensional space

(1) Calculate the rotational energy for first five energy level.

(2) What will be the frequency and wave length of light absorb when transition takes from ground state to first excited state.

(Given: Radius (r)=1.6 Å , h= 6.626×10^{-34} JS, C=3×10^{8} m/sec)

OR

Q.4. B. Answer the following.

1. Explain the total wave function for H-like atom. **[3]**

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

Q.5.A. Derive the radial equation $R = N\rho^{l}L_{(\rho)}\, e^{-\rho/2}$ for H- like atom **[6]**

Q.5.B. Explain time independent theory for non-degenerate system. Also find out first and second order perturbation energy equation. **[6]**

OR

Q.5.B. Answer the following. **[6]**

(i) Discuss the commutation with Hamiltonian.

(ii) Explain Hatree self consistent field method.

Q.6.A. Explain: Born Oppenheimer approximation and derive the electronic and nuclear Schrodinger equation. **[6]**

Q.6.B. Derive the term symbol for the following. **[6]**

(i) He_2 (ii) N_2^{+} (iii) O_2

OR

Q.6.B. Derive the equation $E = 2E_H + 1/R + (j-k) / 1+S$ for hydrogen molecule on the basis of MOT. **[6]**

—X—