SC

No. Of Printed Pages: 2

[46 & A-39]

SARDAR PATEL UNIVERSITY
M.Sc. (SEMESTER-I) EXAMINATION
Monday, 4th April, 2016
10:30 A.M. to 01:30 P.M.
CHEMISTRY: PS01CCHE01
(INORGANIC CHEMISTRY-I)

Note:-figures to the right indicate full marks: **Total marks: 70**

Que : 1 Answer the following: **[8]**

1. When electrons are free in atoms and molecules they undergo _____motion?
   (a) linear (b) Vibrational (c) Rotational (d) None of them
2. Exact solution of Schrodinger equation is possible in simple _____ system only?
   (a) Two electron (b) One electron (c) Many electron (d) None of them
3. Which of the following indicates no degenerate states?
   (a) E_{112} (b) E_{212} (c) E_{222} (d) E_{221}
4. Born Openheimer approximation is very reliable for ____electronic state.
   (a) Excited (b) Both a & b (c) None (d) Ground
5. An angel own as between rotational axis and Z-axis known as...
   (a) θ angle (b) Rotational angle (c) Zenith angle (d) Azimuthal angel
6. The term symbol for n=3, l=2 and s=1 system is....
   (a) $^1D_4, ^1D_3, ^1D_2$ (b) $^3D_3, ^3D_2, ^3D_1$ (c) $^3P_3, ^3P_2, ^3P_1$ (d) $^3D_2, ^3D_1, ^3D_0$
7. The term symbols for B_2 molecule is:
   (a) $^3\Sigma_g$ (b) $^3\Pi_u$ (c) $^2\Sigma_g$ (d) $^3\Sigma_u$
8. H like systems is characterized by
   (a) $+ Ze^2/(4\pi\varepsilon_0)r$ (b) $- ½ Ka^2$ (c) $+ ½ Ka^2$ (d) $- Ze^2/(4\pi\varepsilon_0)r$

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

1. Derive the Schrödinger's equation for particle in one dimensional harmonic oscillator.
2. Derive second order perturbation energy equation.
3. Determine L, S, J & term symbol arising out of coupling between an electrons in S-orbital and another in P-orbital.
4. Determine the value of associated Laguerre polynomial for n=2 and l=1 system.
5. Show that: $\hat{P}x = \pm h/2\pi i \cdot d/dx$
6. Explain the ionic contribution for hydrogen molecule on the basis of VBT.
7. Write a note on Hamiltonian operator.
8. Explain the symmetric and asymmetric wave function.
9. Derive n^{th} order perturbation energy equation.

Que: 3 (A) Butadiene contains 4π electron each of which moves freely from one end of the molecule to the other. Treat the molecule as a one dimensional box whose box length is equal to the length of carbon chain plus half C-C bond length on either other sides. The average C-C bond length is 0.14×10^{-7} cm^{-1}. **[6]**

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

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

(**Given** : h= 6.626×10^{-34} JS, 1J = 6.24×10^{18} eV and 1eV = 8.06×10^3 cm^{-1})

Que: 3 [B] Answer the following:

(I) Show that [Lx, Ly]≠0. **[3]**

(II) Explain the commutation with Hamiltonian. **[3]**

OR

Que: 3 [B] Write a note on quantum mechanical tunneling and write its two applications. **[6]**

Que: 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. (force constant)

(ii) Calculate the lowest vibration energy level.

(iii)Calculate the energy gap between two levels.

OR

Que: 4 [B] Answer the following:

I) Explain the rotational motion of a particle on sphere **[3]**

II) Derive the associated Languerre polynomials for 3d orbital. **[3]**

Que :5 [A] Derive the overall wave function for many electron system. **[6]**

[B] Answer the following:

I) Explain the principle of variation method and derive the equation $E = a_1^2 E_1 + a_2^2 E_2$. **[3]**

II) Calculate the total energy and ionization energy of the He atom in presence and absence of repulsion energy and compare with experimental value. [1a.u.= 0.435×10^{-17}js and 1 joule= 6.24×10^{18} ev.] **[3]**

OR

[B] Write the three conditions for perturbation theory. Explain the first order correction to wave function and second order correction to energy of the eigen function. **[6]**

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

[B] (I) Discuss the adiabatic and crude Born Oppenheimer approximation. **[3]**

(II) Explain LCAOMO treatment for diatomic molecule.

OR

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

****