[31] SEAT No._____ No. Printed pages:3

SARDAR PATEL UNIVERSITY
M.Sc. (SEMESTER-II) EXAMINATION
2019
MONDAY, 18th MARCH
10.00 a.m. to 01.00 p.m.
CHEMISTRY: PS02CCHE21
(QUANTUM CHEMISTRY)

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

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

1. The commutator $[L_+, Lx]$ is equal to:

   a. $\hbar \hat{L}_+$ b. $+\hbar \hat{L}z$ c. $-\hbar \hat{L}z$ d. $-\hbar \hat{L}$.

2. In which of the following situation, quantization can be observed?
   a. Size of the particle is large.
   b. Size of the box is wider.
   c. Wavelength of emitted light is less.
   d. Wavelength of absorbed light is more.

3. What will be effect on the bond strength, if H-atom in C-H bond is replaced by T (tritium) to form C-T bond?
   a. Bond strength increasing
   b. Bond strength remain same
   c. Bond strength decreasing
   d. Bond cannot formed

4. The value of associated Laguerre polynomials for n =2 and l = 1 system is:
   a. 6 b. 1 c. - 6 d. - 1

5. The number of term in series for l=1 and s= 3/2 system is:
   a. Four
   b. One
   c. Two
   d. Three

6. The value of ionization potential energy of helium atom in presence of repulsion energy term is:
   a. -2.75 a.u.
   b. -4.0 a.u.
   c. 0.75 a.u.
   d. 2.00 a.u

7. The value of spin multiplicity for O_2 molecule is:
   a. Four
   b. One
   c. Two
   d. Three

2.....

8. The term symbols for B_2^+ molecule is:

a. $^2\pi_g$ b. $^2\pi_u$ c. $^2\Sigma_g$ d. $^2\Sigma_u$

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

1. Show that, if two operators are commute then they have same set of eiganfuction.
2. Comments on quantization for a particle of mass $1x10^{-30}$kg in a box of length 1Å.
3. Calculate the energy gap and lowest energy of vibrational motion of a C=C in a one dimensional harmonic oscillator. (νC=C = 1675 cm^{-1})
4. Calculate the strength of C-H bond.(νC-H = 3100 cm^{-1})
5. Derive the third order perturbation energy equation.
6. Calculate the total energy of the helium atom in presence and absence of repulsion energy term.(Given: 1 a.u. = $0.435 x10^{-17}$ Js. and 1J = $6.24 X 10^{18}$ eV)
7. Explain the bonding in LiH on the basis of valence bond treatment.
8. What are the conditions for the combination of atomic orbitals?
9. Explain the bonding in HeH.

Q.3.A. Answer the following: **6**

1. Explain the commutative property and show that square of angular momentum operator ($\hat{L}^2$) commute with component of angular momentum operator ($\hat{L}x$).

2. What will be effect on set-down and set-up operators on eiganvalue of component of angular momentum operator and square of angular momentum operator?

B. Explain the utility of particle in box model and calculate the following parameters for the pentadiene molecule: **6**

1. Lowest absorption frequency in cm^{-1}.
2. Wave length of light absorbed in nm.
3. Total ground state energy in cm^{-1}.

[Given: h=$6.626 X 10^{-34}$ Js., 1J = $6.24 X 10^{18}$ eV and 1 eV = $8.06 X 10^3$ cm^{-1}. The length of the pentadiene is equal to the length of carbon chain plus half the C-C bond length on either side and average C-C bond length is $0.14 x 10^{-7}$ cm^{-1}]

OR

B. Answer the following:

1. Define eiganvalue equation and give the list of first four eiganfuction along with eiganvalue for a particle in a box.
2. A system is represented by orthonormal function $\Psi = \sqrt{\frac{2}{9}}\Phi_1 + \sqrt{\frac{7}{9}}\Phi_2$. What are probability of getting the value of energies E_1 and E_2 as an eiganvalue of Φ_1 and Φ_2, respectively?

Q.4.A. Answer the following: **6**

1. Derive the total energy of harmonic oscillator and Schrödinger equation for the vibrational motion of a particle in a one dimensional harmonic oscillator.
2. Derive the first, second and third degree of Hermite's polynomials.

3....

B. Answer the following: 6

1. Calculate the first three angular momentum and first three energy levels for the rotational motion of NO molecule in three dimension and xy-plane.
   [Given: $r = 1.15 \times 10^{-10}$ m].
2. Derive the normalization factor of the wave function for a one dimensional harmonic oscillator and rotational motion of a particle.

OR

B. Find out the value of the Laguerre polynomials, associate Laguerre polynomials and normalization factor (N) for n = 2, l = 0 and n = 3, l = 1 systems.

Q.5.A. Define Dirac notation. What are the conditions for the perturbation treatment? Discuss the variation method for estimating the energy and approximating wave function. 6

B. Answer the following: 6

1. Explain the self-consistent field method for obtaining better wave function.
2. Derive the term symbols arising out of the coupling between an electron in f-orbital and an electron in g-orbital.

OR

B. Discuss the wave functions for the many electron systems.

Q.6.A. Answer the following: 6

1. Differentiate the π- MO's and σ-MO's and explain the order of molecular energy levels for N_2^+ and F_2^+ molecules.
2. Determine the coefficient a_1 and a_2 and explain the electron density distribution in hydrogen molecule on the basis of valence bond treatment.

B. Answer the following: 6

1. Derive the equation $E_1 = \frac{HAA+HAB}{1+S}$ for hydrogen molecule ion on the basis of molecular orbital theory.
2. Determine the term symbols for the C_2^+, F_2^+ and O_2^+ molecules.

OR

B. Derive the equation $E_1 = 2E_H + \frac{1}{R} + \frac{J+K}{1+S^2}$ for hydrogen molecule on the basis of valence bond theory.