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SEAT No._____

No. Printed pages:3

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SARDAR PATEL UNIVERSITY
M.Sc. (SEMESTER-I) EXAMINATION
2017
Wednesday, 1st November
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. Due to effect of set down operator, eigenvalue of angular momentum operator ($\hat{L}z$) is:
   a. Decrease by ħ b. Increase by ħ
   c. Remain same d. Increase by ħ/2

2. Due to distortion along y-axis, energy of the state E_{221} is decrease by:
   a. $-\frac{h^2}{ML^2}$ b. $-\frac{h^2}{ML^3}$ c. $-\frac{h^2}{4ML^2}$ d. $-\frac{h^2}{4ML^3}$

3. The boundary condition for the rotational motion of particle are:
   a. 0 to L b. 0 to π c. 0 to 2π d. - L/2 to + L/2

4. The value of associated Laguerre polynomials for n =1 and l = 0 system is:
   a. 6 b. 1 c. - 6 d. - 1

5. The expression for the fourth order perturbation energy is:
   a. $< \psi^1 | \hat{V} | \psi^2 >$
   b. $< \psi^2 | \hat{V} | \psi^2 >$
   c. $< \psi^0 | \hat{V} | \psi^3 >$
   d. $< \psi^0 | \hat{V} | \psi^4 >$

6. The value of ionization energy of helium atom in presence of repulsion energy term is:
   a. -2.75 a.u.
   b. -4.00 a.u.
   c. 2.00 a.u.
   d. 0.75 a.u

7. Which of the following symbol is used for the overlap integral?
   a. H_{AB}
   b. S_{AB}
   c. S_{AA}
   d. H_{AA}

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8. The value of spin multiplicity for F_2^+ molecule is:
   a. Four
   b. One
   c. Two
   d. Three

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

1. What are the application of quantum mechanical tunneling?
2. Evaluate the commutator $[Z, \frac{\partial}{\partial z}]$.
3. Explain the total wave function for hydrogen like atom.
4. Derive the kinetic energy of harmonic oscillator.
5. Derive the first order perturbation energy equation.
6. Calculate the total energy of helium atom in presence and absence of repulsion energy term.(Given: 1 a.u. = 0.435×10^{-17} Js. and 1J = 6.24×10^{18} eV)
7. Explain the bonding in LiH on the basis of valence bond treatment.
8. The $\pi_u 2Px$ orbital is higher in energy than $\sigma_g 2Pz$ for the F_2 system. Explain.
9. Explain the eigenvalue equation.

Q.3.A. Show that square of angular momentum operator ($\hat{L}^2$) commute with component of angular momentum operator ($\hat{L}x$) and shift operator ($\hat{L}_+$), while component of angular momentum operator ($\hat{L}x$) does not commute with component of angular momentum operator ($\hat{L}y$) and ladder operator ($\hat{L}_+$). **6**

B. Explain the utility of particle in box model and calculate the following parameters for the butadiene 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=6.626×10^{-34} Js., 1J = 6.24×10^{18} eV and 1 eV = 8.06×10^3 cm^{-1}. The length of the butadiene 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 0.14×10^{-7} cm^{-1}]

OR

B. Answer the following:

1. Derive the equations for Hamiltonian and angular momentum operators.
2. Derive the wave function and energy equation for a translational motion of a free particle. **6**

Q.4.A. Answer the following:
1. Derive the value of normalization factor (N) of the radial eiganfunction for n = 1, l = 0 and n = 3, l = 1 systems.
2. Derive the third degree of Hermite's polynomial.

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B. Answer the following: 6

1. Derive the Schrödinger equation for the vibrational motion of a particle in a one dimensional harmonic oscillator.
2. Derive the normalization factor and the characteristic of eiganfunction of a one dimensional harmonic oscillator.

OR

B. Answer the following:

1. Derive the recursion formula for the Hermite's differential equation.
2. Explain the rotational motion of particle on a sphere.

Q.5.A. Explain the Dirac notation and discuss the time independent perturbation theory for non-degenerate case. 6

B. Explain the spin-orbit interaction Derive the term symbols arising out of the coupling between an electron in d-orbital and an electron in f-orbital. 6

OR

B. Answer the following:

1. Discuss the Hatree-self consistent field methods.
2. Derive the equation for the first order correction to wave function.

Q.6.A. Discuss the Born- Oppenheimer approximation for the solution of Schrödinger equation. 6

B. Explain the MO theory of bonding for hydrogen molecule. 6

OR

B. Answer the following:

1. Explain the electronic state and term symbols for diatomic molecule. Determine the term symbols for the Be_2, N_2^+ and O_2^+ molecules.
2. Explain the bonding in HeH and He_2 molecules

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