SL

No. Printed pages: 3

(21) **SARDAR PATEL UNIVERSITY**

M.Sc. (SEMESTER-1) EXAMINATION

2015

Saturday, 18th April

10:30a.m. to 1:30p.m.

CHEMISTRY:- PS01CCHE01

(INORGANIC CHEMISTRY-1)

Note:- Figures to the right indicates full marks. **Total marks:-70**

Q-1 Answer the following: **[8]**

1. Which of the following is the correct relation between Cartesian and Polar coordinates?
   (a) $x=r \sin\Phi \cos\Phi$; $y=r \sin\Phi \sin\theta$; $z=r \cos\theta$
   (b) $x=r \sin\theta \cos\Phi$; $y=r \sin\Phi \sin\theta$; $z=r \sin\Phi$
   (c) $x=r \sin\Phi \cos\theta$; $y=r \sin\Phi \sin\theta$; $z=r \sin\theta$
   (d) $x=r \sin\theta \cos\Phi$; $y=r \sin\theta \sin\Phi$; $z=r \cos\theta$
2. The free electrons in an atoms & molecules can execute_____ Motion.
   (a) Rotational (b) Vibrational (c) Linear (d) None
3. In H_2^+ ion the bond distance and bond dissociation energy is _____ & _____ respectively.
   (a) $1.60A^0$, 2.97 eV (b) $1.79A^0$, 2.06 eV
   (c) $1.06A^0$, 2.69 eV (d) $1.06A^0$, 2.8 eV
4. Which of the following indicates non degenerate states?
   (a) E_{112} (b) E_{212} (c) E_{221} (d) E_{222}
5. The Commutator [Lz, L_+] is equal to
   (a) $\hbar L_+$ (b) $\hbar L_-$ (c) $-\hbar L_+$ (d) $-\hbar L_-$
6. Born Open heimer approximation is very reliable for_____ electronic state.
   (a)Ground (b) Excited (c) Both a & b (d) None
7. An angel between rotational axis and Z-axis known as
   (a) Azimuthal angel (b) Rotation angle
   (c) Zenith angel (d) θ angle
8. In vibrational motion of particle, as n increases the energy gap also_____.
   (a) Increase (b) Decrease (c) constant (d) none of these

Q-2 **Attempt any SEVEN** **[14]**

1. Find out 3rd degree of polynomial.
2. Show that Py = -h/2πi d/dy
3. S.T the average kinetic energy is equal to E.
4. Calculate the energy of state E_{211} by distortion along X-axis and show the effect of distortion on energy.
5. Write a note on Hamiltonian operator.
6. Determine L, S, J & term symbol arising out of coupling between an electrons in S-orbital & another in P-orbital.
7. Determine the value of associated laguerre polynomial for n=3 & l=2.
8. S.T component of angular momentum operator Lx does not commute with set down operator.
9. Find out the normalization factor for the rotational motion of a particle.

Q-3(A) Butadiene contains 4π electrons, 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 C-C bond plus half the C-C bond length on either side. The average C-C bond length is 0.14nm. **[06]**

(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})

Q-3(B) Explain Quantum mechanical tunneling. **[06]**

OR

Q-3(B) **Answer the following:**

1. Explain square of angular momentum and its component (X, Y) Commute with each other. **[03]**
2. Discuss the translational motion of a cubical box. **[03]**

Q-4(A) Assuming harmonic oscillator model for C-C, C=C and C≡C with frequency 1400cm^{-1}, 1700 cm^{-1}, 2100cm^{-1} respectively. Calculate bond strength, lowest vibrational energy and energy gap between two levels. **[06]**

Q-4(B) Considering CO as a rigid rotator rotates in a (I) XY-plane (II) 3-dimension: **[06]**
(i) Calculate the frequency and wavelength of light emitted when transition takes place from excited state to ground state i.e., n=1 to n=0.
(ii) Calculate the angular momentum and first three rotational energy level.
(**Given**: Radius (r) =$1.x10^{-10}$ m, h= 6.626×10^{-34} JS, C=3×10^{8} m/sec)

OR

Q-4(B) Answer the following:

1. Explain Rotational motion of diatomic molecules can occur in a plane (Fixed axis) **[03]**
2. Derive radial eigen function for n=1 and l=0 system. **[03]**

Q-5(A) Explain time independent perturbation theory for non-degenerate system. Also find out first and second order perturbation energy equations. **[06]**

Q-5(B) Derive Overall wave function for many electron systems. **[06]**

OR

Q-5(B) Answer the following:

1. State the principle of variation method and derive, $\mathbf{E} = a_1^2\mathbf{E}_1 + a_2^2\mathbf{E}_2$. **[03]**
2. 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 ×1018 ev.] **[03]**

Q-6(A) Derive the energy equation $\mathbf{H_{AA} = 2E_H + 1/R + J}$ for hydrogen molecule on the basis of Heitler- London theory. **[06]**

Q-6(B) M. O. Theory of bonding in H_2 Molecules. **[06]**

OR

Q-6(B) Answer the following:

1. Discuss the LCAOMO treatment of diatomic molecules. **[03]**
2. Explain bonding in HeH on the basis of VB treatment. **[03]**

ALL THE BEST