**Geo – Chemist Test Series (P – 6)**

 **Syllabus: - Quantum , and molecular Spectroscopy**

**Marks: - 200**

**Time Allowed: - 3/hrs**

 **Section – A (Compulsory Section)** (5x16)

1. (a) Calculate angular momentum of 1s, 3p, 4d, and 7g orbitals.

(b) Which of the three vibration of an *AB*2 molecule are infrared or Raman active if it is (i) linear (ii) angular.

 (c) Discuss the 1H – NMR of pure ethanol and acidified ethanol.

 (d) Justify the following statements:

1. Fluorescence is favoured at very low pressures,
2. Phosphorescence, unlike fluorescence, cannot be studied in the liquid phase.

 (e) Show that the function A sin for a particle in a one – dimensional box of length L in not an eigenfuncation of the momentum operator, , but it is so of . Discuss the significance of the result.

(f) If sufficient energy is absorbed by an atom, an electron can be lost by the atom and a positive ion formed. The amount of energy required is called the ionization energy. In hydrogen atom, the ionization energy is that required to change the electron from n = 1 to n = ∞. Calculate the ionization energy (in KJ mol-1) for Li+2 ions. Is the ionization energy Li+2 ion more or less than that of hydrogen?

 (g) Which of these functions is /are Eigen factions of the d/dx operator?

i) Exp (ax). ii) exp (ax2), (iii) sin (x), (iv) 25 x2

(h) Name a particle having both wave and particle properties, state uncertainty principle. Can uncertainty principle be applied to flying Jet Plane? Why?

(i) Calculate the de Broglie wave length of an electron that has been accelerated by a potential difference of 1000 volts.

(j) The fundamental vibrational frequency and rotational cons taint of co molecule are 6.5 x 1013 s-1 respectively. Find the rotational quantum for which co molecule will have some energy as it would have in its first vibrational state with no rotational energy.

(k) Classify the molecule as microwave active & in active.

H2 HCl, CH4 H2O, CO2 N2 NO2 N2O.

 (l) Derive the relationship for Jmax of a diatomic molecule.

(m) What is the interpretation of (wave function) and (square of wave equation).

(n) What is zero point energy of SHO. In which case ZPE is higher H2O or CH4 explain.

(o) What are degeneracies of the following orbitals for hydrogen-like atoms (i) 1s (ii) 2s (iii) 2p

(p) Compare and the force constant for CN and CN+ if vibrational frequency are 2068.61 cm-1 & 1580 cm-1 respectively. Interpret the result on basis of electronic configuration.

 **Section – B**

Attempt any three questions

1. (a) The wave functions for a particle in a one-dimensional box (length L) are



 Calculate the uncertainty in position. (5)

(b) Zero point energy of Cl2 molecule is 2x10-21 J calculate force constant assuming it behave like SHO. (5)

1. The vibrational wave number of the following molecules in their are HCl (2885 cm-1); DCl (1990 cm-1); D2 (2990 cm-1); and HD (3637 cm-1) Calculate the energy change, in KJ mol-1 of the reaction  (10)
2. The basic Schrödinger equation for a hydrogen (l-electron) atoms is



 i) Explain what the terms in this equation means.

1.  is the reduced mass of the electron –nucleus pair. For hydrogen, how does it compare with me, the mass of the electron?
2. Evaleuate the average electon –nucleus separation for the ground state of a hydrogenic atom:

 And the waveefunction is given by





Where Z is the nuclear charge and is the Bohr radius.

1. Why is this different from the msost probable radius (a0/Z)? (10)
2. (a) Show that, for a free particle moving in an unbounded region of space, the translational energy is virtually unquantized. (3)

(b) To what temperature must we heat a diatomic gas at 298 K to excite one percent of its molecule to the first excited state of vibrational energy level. The fundamental frequency of gas is 1545 cm-1. (7)

1. The harmonic oscillator model provides a means of interpreting the vibrations of small molecules, when applied to photonuclear diatomic molecule made up of atoms with mass m, the model yields vibrational energy levels given by

En = 

 Where n = 0, 1, 2, ………is the vibrational quantum

 Number, k is the force constant reduced mass.

1. Sketch an energy level diagram for the harmonic oscillator, showing the four the first four energy levels in units of .
2. The ground state wave function for the harmonic oscillator is given by



Where x is the deviation from equilibrium bond separation and sketch the wave function and then determine the most probable value of x and the average value of x.

1. The vibrational wave number of diatomic chlorine, 35Cl2, is 559. 71 cm -1  calculate the force constant for the Cl – Cl bond. Assuming that the atomic weight of Cl is exactly 35. (10)
2. Define and differentiate between the following:

i) Normalized and Orthogonal wave functions

ii) Eigen value and Eigen function

1. Eigen value and Most probable value (10)
2. (a) Explain concisely what is meant by nuclear spin – spin coupling using the 1H NMR spectrum of CHBr2 CHO as an example. Explain how spin – spin coupling arises in this example.

 (b) What is meant by the tem coupling constant (J)?

1. (a)  (5)

(b) Write down the Hamiltionian for the hydrogen molecular ion, H2+ (5)

 **Section – C**

Attempt any three questions.

1. The Bohr model for single-electron atoms predicts that the energies of the allowed orbitals are given by



Where n =1, 2, 3, …., and z is the nuclear charge.

1. The Balmer sericese corresponds to transitions between which energy levels in the hydrogen atom? Does the paschen series appear at higher or lower wavelengths than the Balmer series?
2. Calculate the minimum energy (in J) required to ionize an electron in the n =2 state of hydrogen atom.
3. Calcualte the wavelenght (in nm) of the photon emitted by an electron in making the transition from the n =3 to n = 1 level fo the single –electron ion, Li2+,
4. Is the photon higher in energy or lower in energy than the transition from n =3 to n =1 in Be3+? Explain your answer. **5+5+5+5**
5. (a) (i) HCl molecules absorb radiations of wavelength 2909.5 cm-1. Calculate the accompanying change in internal energy of an HI molecule in Joule. (5)

(ii) Determine the number of normal vibrational modes of each of the following molecules: hydrogen chloride; hydrogen cyanide, ethane benzene. (5)

(iii) Deduce which of the following molecules will show a microwave (rotational) spectrum and explain your answer:

 Br2; NO; O2 (3)

 (b) What are Rayleigh, stoke and anti – Stokes lines? Is the intensity of Stokes lines different from that of the anti – Stokes lines? Explain. (3)

 (ii) Sketch the normal modes of vibration of CO2 and explain which of these Raman is and which are IR active. (4)

1. (a) The vibrational energy levels of I2 molecule is given by calculate (a) force constant of bond (b) anharmonicity constant (c) zero point energy (d) fundamental & first overtone frequency (e) quantum number which leads to dissociation (f) dissociation energy. (12)
2. Draw the radial part of the wave function and radial probability distribution for hydrogen atoms for 1s, 2s and 2p orbitals. (8)
3. (a) The separation between successive lines of rotational spectrum of a distance molecule is 20 cm-1. Calculate (i) moment of inertia (b) which rotational level have highest population. (8)

(b) A particle of mass m is confined in a one –dimensional box if length L. the wave functions  of the particle are given by



n is the quantum number, and  is the distance along the length of the box.

1. Sketch the waveefunctions for the states with n =1, n=2 and n=3.

(ii) Describe what is meant by the Born interpretation,



(iii) Sketch the probability of finding the partcile within the box for the states with n =1, n=2 and n=3.

1. What is the averge momentum of a partile in a box? (12)