17P112 (Pages:2) Name: .....

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, DECEMBER 2017

(Regular/Supplementary/Improvement)

(CUCSS-PG)

CC15P CH1C01 – BASIC CONCEPTS IN QUANTUM CHEMISTRY AND GROUP THEORY

(Chemistry)

(2015 Admission Onwards)

Time: Three Hours Maximum: 36 Weightage

PART - A

Answer ***all*** questions. Each question carries 1 weightage.

1. Determine whether the following functions are acceptable or not over indicated intervals

   a) e^{-x} (x varies from $-\infty$ to ∞) b) $\sin^{-1} x$ (x varies from -1 to 1)
2. What is spherical harmonics? Give two examples.
3. What is a radial distribution function? Sketch radial distribution plots for 2s and 3p orbitals.
4. A particle is confined in a potential box of width 10 Å . If the zero point energy is 0.6×10^{-12}erg. Calculate the mass of the particle
5. The state of a system is described by $\psi(x,t)$which is a function of both position and time, but the average value of any physical quantity is independent of time. Why?
6. What is orthonormal function?
7. The product of two reflections is a rotation" Justify
8. What is rearrangement theorem? .Apply this theorem to construct the GMT for C_4 point group.
9. What is Paulis Principle of antisymmetric wave functions?
10. What are the distinct operations generated by S_3 axis?
11. Generate the matrix for C_4 and i operations.
12. Show that all cyclic groups are abelian.

(12 x 1 = 12 weightage)

PART -B

Answer any ***eight*** questions. Each question carries 2 weightage.

13. Derive the Schrodinger wave equation from classical wave mechanics
14. Find the eigen values and eigen functions of a particle in three dimensional box. Explain the term degeneracy.

15. Derive the wave functions in real form for the particle on a ring from the wave equation in spherical polar coordinates.
16. Discuss the utility of one dimensional box in the interpretation of electronic spectra of conjugated organic molecules.
17. State Great Orthogonality theorem.Discuss its properties
18. Derive reduction formula.What is its application.
19. 19. Show that $\angle^2$ commutes with $\angle_z$ ($\angle$ is operator for angular momentum)
20. Show that (i,-i,1,-1) obey the properties of a mathematical group .
21. List the symmetry elements and symmetry operations of C_{2h} and find out the classes
22. Assign schoenflies symbol for the point group of following molecules:-

    i) Ferrocene ii) cyclohexane (chair) iii) Naphthalene iv) BF_3

    v) NH3 vi) HCl vii) Ethylene viii) Allene
23. State and explain the spin postulate by Uhlenbeck. What is a spin orbital?
24. List the symmetry elements and symmetry operations in C_{4v} and construct its group multiplication table.

(8 x 2 = 16 weightage)

PART -C

Answer any ***two*** questions. Each question carries 4 weightage

25. Derive the Schrodinger equation and solve it completely for one dimensional box. Sketch probability plots.
26. Construct the character table of C_{3v} point group.
27. Apply Schrodinger equation for a harmonic oscillator. Find eigen values and eigen functions. Sketch the wave functions.
28. Apply Schrodinger equation for non planar rotator. Transform it into spherical polar co-ordinates and separate the variables and solve for theta equation.

(2 x 4 = 8 weightage)

****