

Name: .....

Reg. No.....

FIRST SEMESTER M.Sc. DEGREE EXTERNAL EXAMINATION FEB. 2016

(2015 Admission)

**CC15P CH1C01 – Basic Concepts in Quantum Chemistry and Group theory**

(Chemistry)

**Time: Three hours****Maximum weightage: 36****Section A**(Answer **all** questions. Each question has 1 weightage)

1. A wave function is given by  $\psi = \sin x$ . Is it acceptable? Is it normalized? Explain.
2. What are spherical harmonics? Write two examples.
3. Define Hermitian operator.
4. What is Ladder operator? What is its significance?
5. Write a general expression for Legendre polynomials. Find out the Legendre polynomials when  $l=0,1,2$ .
6. What is recursion formula? Give its significance.
7. What is inverse and conjugate of an operator? Give examples.
8. Give the number of irreducible representations of the  $C_s$  point group and obtain their dimensions.
9. Give the product of  $C_2^x \sigma_{xy}$  using matrix representations.
10. What are the distinct operations generated by  $C_6$  axis?
11. What are representations? Construct a representation using  $p_x$  and  $p_y$  orbitals as basis for a  $C_{2v}$  point group.
12. What do  $A_{2u}$  and  $B_{2g}$  representations mean?

**(12 x 1 = 12 weightage)****Section B**(Answer **any 8** questions. Each question carries 2 weightage.)

13. Discuss the postulates of quantum mechanics.

14. Discuss the features and significance of solution of one dimensional box.
15. Find the eigen values and eigen functions of a particle in three dimensional box. Explain the term degeneracy
- 16 Calculate the average value of momentum of a particle confined to one dimensional box of length 'a'
17. State and explain the spin postulate by Uhlenbeck. What is a spin orbital?
- 18 Taking a suitable example illustrate the properties of a mathematical group.
19. Derive the Group multiplication table for  $C_{2h}$  point group
20. Construct a representation for ammonia taking all the Cartesian coordinates of atoms as basis.
- 21 Assign the symmetry operations in a  $D_{3h}$  point group taking a suitable example
- 22 .State Great Orthogonality theorem. Discuss its properties
23. What is similarity transformation? Find out the classes in a  $C_{2v}$  point group.
24. Derive the wave functions in real form for the particle on a ring from the wave equation in spherical polar coordinates **(8 x 2 = 16 weightage)**

### Section C

(Answer **any 2** questions. Each question carries 4 weightage)

25. Apply Schrodinger equation for a harmonic oscillator. Find eigen values and eigen functions. Sketch the wave functions
26. Apply Schrodinger equation for H atom. Transform it into spherical polar co-ordinates and separate the variables and solve for radial equation.
27. Show that the square of the angular momentum and its z component can be specified simultaneously. Discuss space quantization.
28. Construct the character table of  $C_{4v}$  point group **(2 x 4 = 8 weightage)**

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