FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2018
(Regular/Supplementary/Improvement)
(CUCSS-PG)
CC15P CH1 C01 – BASIC CONCEPTS IN QUANTUM CHEMISTRY AND GROUP THEORY
(Chemistry)
(2015 Admission onwards)

Time: Three Hours   Maximum: 36 Weightage

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

1. Differentiate between abelian and non-abelian groups with examples.

2. The degeneracy of a cubical box is lifted by making the sides in different length. Exemplify.

3. Calculate the probability that a particle in one dimensional box of length 'a' is found to be between   (i) 0 and a/2   (ii) 0 to a.

4. What you mean by orthonormality?

5. Draw the polar diagram of $Y_0^0 = (1/4\pi)^{1/2}$ and $Y_1^0 = (3/4\pi)^{1/2} \cos\theta$

6. Prove that spherical harmonics is an eigen function of angular momentum.

7. Briefly explain ladder operators.

8. Explain the term tunnelling and space quantisation.

9. What are spin orbitals?

10. Assign schoenflies symbols for a point groups of following molecules.

    (i) Allene   (ii) Dichloromethane

11. List the symmetry operations of D_{3h} taking BF_3 as an example.

12. State and explain Uhlenbeck spin postulate.

(12 × 1 = 12 Weightage)

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

13. Derive the wave function and energy of a particle in a 3D box.

14. Calculate the average value of momentum and energy for a particle in 1D box.

15. Deduce the polynomial solution for a vibrating diatomic molecules suggesting simple harmonic oscillator character.

16. Find the commutator [Lx, Ly]

17. Generate the group multiplication table for C_{3v}.

18. Show that L^2 commutes with L_z.

19. Define hermitian operator. Show that hermitian operator always have real eigen values.

20. Show that the symmetry operations, E, $C_{2(Z)}$, i and σ_{xy} form a mathematical group.

21. Calculate the legendre and associated legendre polynomials of

$$P_0^0(x), P_1^0(x), P_1^1(x), P_2^0(x), P_2^1(x), P_2^2(x)$$

22. Derive the wave function for a planar rigid rotator.

23. Check whether C_{2v} point group is a cyclic group.

24. Write the matrices for C_3 and S_3 operations.

(8 × 2 = 16 Weightage)

Section C

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

25. State and explain the great orthogonally theorem. What are the consequences of the theorem?

26. Discuss the systematic procedure to assign Schoenflies symbol for a point group.

27. (i) Briefly explain the postulates of quantum mechanics.

(ii) Derive the solution of radial equation for hydrogen like atoms.

28. (i) Deduce the schrodinger equation for classical wave equation.

(iii) Clarify the significance of quantum theory with the aid of black body radiation and photoelectric effect.

(2 x 4 = 8 Weightage)

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