16P110 (Pages:2) Name: …….
Reg. No……

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2016

(Regular/Supplementary/Improvement)
(CUCSS-PG)

CC15PCH1C01 – 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 has* 1 *weightage*)

1. The solutions for a planar rotator is given by $\varphi = \frac{1}{\sqrt{\pi}} e^{im\phi}$ (m=0, ±1, ±2……). Express the solutions as real functions.
2. Show that eigen functions of a rigid rotor are also eigen functions of $L^{\wedge 2}$ operator
3. Write complete wave equation for an electron in the state *n*=1, *l*=0, *m*=0
4. Write recursion formula. Explain its significance.
5. Write associated Laguerre equation. Explain the terms
6. Define the term degeneracy of an energy level. Calculate the degeneracies of a particle in a 3D cubical box having energies equal to i) 6 and ii) 14 in units of $h^2/8ma^2$
7. What do you mean by polar plot. Draw one polar plot.
8. Show that wave function $\psi_{(1)\,x}$ for SHO is normalized.
9. Write the matrices for C_3, C_3^2, S_4 operations.
10. What meaning is implied in the Mulliken symbols A_1, A_2 and E in C_{3v} point group?
11. Distinguish between conjugate operations and inverse operations.
12. What is an abelian group? Give one example.

(12 × 1 = 12 weightage)

Section B

(Answer any 8 *questions. Each question carries* 2 *weightage)*

13. Derive the wave equation for particle on a ring.
14. Write associated Legendre equation. What are its solutions? Write equations for Legendre polynomials and the normalization constant.
15. 1s wave function of H atom is $\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-(r/a_0)}$. Show that maximum probability to find the electron is at r = a_0.
16. Find the commutator [Lx, Ly]
17. Explain quantum mechanical tunneling.
18. Calculate the expectation value for kinetic energy for $\psi_{(0)}$ for SHO.

19. Evaluate $|\Delta E| . |\Delta t|$. Also find the life time of the excited state species if the width of the spectral line is 0.15 cm^{-1}
20. Calculte the expectation value $<p_x>$ for particle in one dimensional box for n = 1. Comment on the result.
21. What is meant by 'class' in a mathematical groups? Prove that three vertical planes in ammonia molecule belong to same class.
22. Determine the point groups of following molecules (a) pyridine (d) allene (c) staggered and eclipsed ethane (d) chair conformation of cyclohexane
23. Distinguish between reducible and irreducible representations. Give an example for both in a C_{3v} point group.
24. Reduce following reducible representations Γ_a and Γ_b in C_{3v} into irreducible representations. The C_{3v} character table is given.

C_{3v}	E	$2C_3$	3σ
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
Γ_a	5	2	-1
Γ_b	7	1	-1

(8 × 2 = 16 weightage)

Section C

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

25. Apply Schrodinger equation for simple harmonic oscillator. Find eigen values and eigen functions.

26. The R equation for H atom is given by

$$\frac{1}{R(r)}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R(r)+\frac{8\pi^2 m}{h^2}(E+\frac{e^2}{4\pi\varepsilon r})=\beta$$

Solve the equation to find eigen values and eigen functions. (If unfamiliar solve the R equation which you are used to)

27. Prove that a) Eigen values of hermitian operators are real and b) Eigen functions of hermitian operators corresponding to two different eigen values are orthogonal.

28. State and explain great orthogonality theorem (GOT). What are the consequences of the theorem? Using GOT, derive the character table of C_{4v} point group.

(2 x 4 = 8 weightage)

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