Reg. No..... Name: .....

MSC DEGREE END SEMESTER EXAMINATION 2014 -15
SEMESTER -1: CHEMISTRY
COURSE: P1CHET03/P1CPHT03 - QUANTUM CHEMISTRY AND GROUP THEORY

Time: 3 Hrs. Max. Marks: 75

Section A

*Answer any **10** questions.*

1. What is a state function? What are the conditions required for a state function to represent a visible physical state?
2. What do you mean by polar plot? Draw one polar plot.
3. Write wave functions for a simple harmonic oscillator corresponding to $\nu = 0$ and $\nu = 1$ state. Represent it graphically.
4. Write Rodrigue's formula. Explain the significance.
5. What are spherical harmonics? Write first two spherical harmonics.
6. State and explain the postulate of spin by Uhlenbeck.
7. Distinguish between reducible and non-reducible representation with examples.
8. What is a cyclic group? Give an example.
9. Find the direct product $E_g \times A_u$ in C_{2h}. Use C_{2h} character table in Question No.21.
10. Reduce the representation (6 0 -2). Use C_{3v} character table in Question No.25.
11. What are vanishing and non vanishing integrals?
12. Define "normal modes of vibration".
13. State Laporte selection rules for centrosymmetric systems.

(10 x 2 = 20)

Section B

*Answer any **5** questions.*

14. Assume a particle confined to a three-dimensional box having dimensions:
    (i) a = b = c, (ii) a = b ≠ c. Given the quantum number values of 1 and 2. Calculate energies for levels E_{211}, E_{121}, E_{122} and E_{212} and comment on its degeneracy, if any.
15. Show that Hermitian operators always have real eigen values.
16. Write a note on tunnelling effect.
17. Discuss the Stern Gerlach experiment and the corresponding inferences.
18. What is similarity transformation? Illustrate using suitable example.
19. Find E x E. Reduce it into its IR components. Use C_{3v} character table in Question No.25.
20. Generate matrices for C_3 and σ_h and show that their product is an S_3.

21. Using Cartesian coordinates find out the normal modes of vibrations in N_2F_2. Identify the Raman active vibrations. Use C_{2h} character table.

C_{2h}	E	C_2	*i*	σ_h		
A_g	1	1	1	1	R_x	x^2, y^2, z^2, xy
E_g	1	-1	1	-1	R_z, R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x, y	

(5 x 5 = 25)

Section C

*Answer any **2** questions.*

22. Set up the Schrodinger equation for hydrogen atom. Separate the variables and obtain the solution for the *phi* equation.

23. Discuss the ladder operator method to obtain the eigen values for angular momentum.

24. Using Great orthogonality theorem derive C_{4v} character table.

25. Find IR and Raman active vibrations in NH_3. Use C_{3v} character table.

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	-1	R_z	
E	2	-1	0	(x,y) (R_x, R_y)	(x^2-y^2, xy) (xz, yz)

(2 x 15 = 30)

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