Reg. No ..... Name **17P146**

MSc DEGREE END SEMESTER EXAMINATION - NOVEMBER 2017

SEMESTER 1 : CHEMISTRY / PHARMACEUTICAL CHEMISTRY

COURSE : **16P1CHET04 / 16P1CPHT04 - QUANTUM CHEMISTRY AND GROUP THEORY**

(Common for Regular - 2017 / Supplementary - 2016 Admissions)

Time : Three Hours Max. Marks: 75

Section A

Answer any 10 (2 marks each)

1. A reducible representation of C_{3v} point group is given below.

C3v	E	$2C_3$	$3\sigma_v$
T_R	4	-1	0

Split this representation into the component irreducible representations

2. The sigma bonds are used as basis vectors for generating the reducible representation to understand the bonding properties of a molecule. Explain
3. Comment on the complimentarity of the IR and Raman activity of the vibrational modes of a molecule that belong to C2h point group
4. List the symmetry elements and operations of chloroform molecule. What is its point group?
5. Write the multiplication table for C_3 point group? What type of point group is it?
6. What are the properties of Abelian groups? Explain with one example
7. What are eigen functions and eigen values. Give example.
8. Calculate the uncertainty in position of an electron moving with a velocity of 2×10^6 ms^{-1}, accurate upto 0.001 %.
9. Discuss the physical origin of quantisation of energy for a particle confined to move around a ring.
10. Explain the term degeneracy. What is the maximum degeneracy possible for a particle in a cube?
11. Zero point energy of a rigid rotator is zero. Is this against the uncertainty principle?
12. The n =1 to n = 2 absorption frequency for a certain particle in a certain one-dimensional box is 6.0×10^{12} s^{-1}. Find the n =2 to n = 3 absorption frequency for this system.
13. Calculate the average distance of the electron from the nucleus in the ground state of hydrogen atom, given that the normalized ground state wave function is $\Psi_{1s} = (1/\pi a_o^3)^{½} \exp(-r/a_o)$

(2 x 10 = 20)

Section B
Answer any 5 (5 marks each)

14. Determine the symmetries of the vibrational modes of trans-N_2F_2 molecules using internal co-ordinates
15. What are internal co-ordinates? Explain its application in determining the symmetries of the vibrational modes of ammonia molecule
16. Derive the part 1 and 2 of the character table for C_{3v} point group
17. The operations of a point group are {E, $2C_4(z)$, C2, $2C_2'$, $2C_2''$, i, $2S_4$, $2\sigma_v$, $2\sigma_d$}. Identify the point group, order of the group. How many irreducible representations does it have? Can C_{4v} point group be a subgroup?
18. Show that Schrodinger wave equation is an Eigenvalue equation
19. Prove that $[L^2, L_x] = 0$.
20. The force constant of $^{79}Br^{79}Br$ is 240 Nm^{-1}. Calculate the fundamental vibrational frequency and zero-point energy of Br-Br, approximating the molecular vibration as that of a harmonic oscillator.
21. Discuss the radial and angular Schrodinger equation of hydrogen atom depend on the variables r, θ,φ and its solutions

(5 x 5 = 25)

Section C
Answer any 2 (15 marks each)

22. Determine the symmetries of the vibrational modes of ammonia molecule and predict the IR and Raman acitivity based on the selection rules.
23. What are character tables? State the theorem concerning the irreducible representations of a group. And use the theorem to derive the character table for C_{2v} point group.
24. Solve the Schrödinger equation for a rigid rotator. Discuss the results.
25. With the help of diagrams, explain the radial wave function, radial probability density and radial probability distribution function of orbitals corresponds to $R_{1,0}$, $R_{2,0}$, $R_{3,0}$, $R_{2,1}$, $R_{3,1}$, $R_{3,2}$ hydrogen wave functions.

(15 x 2 = 30)