Reg.No..... Name : ..... **P 131**

MSc DEGREE END SEMESTER EXAMINATIONS – NOVEMBER 2015

SEMESTER- 1, SUBJECT: **CHEMISTRY/PHARMACEUTICAL CHEMSITRY**
COURSE: **P1CHET03 / P1CPHT03 QUANTUM CHEMISTRY AND GROUP THEORY**

Time: Three Hours Max. Marks: 75

SECTION A

*(Answer any **10** questions. Each question carries **2** marks)*

1. What is a Hermitian operator? Name one such operator.
2. Sort the following functions into odd and even: a) 9 b) x^2 c) $3x^3$ d) cosx.
3. Given that the energy of a particle of mass 'm' in a cubic box of length L is $9h^2/mL^2$. What are the state functions associated with this energy level? What is the degeneracy?
4. Calculate the quantum number of a particle of mass of 1g in a 10cm length box having energy kT at room temperature.
5. Prove that the nonexistence of zero point energy in planar rigid rotator is not in violation of Heisenberg's uncertainty principle.
6. Justify the choice of spherical polar coordinates for solving Hydrogen like atom.
7. Give the sketches of the radial distribution function for 1s, 2s and 3s orbitals.
8. Explain with examples improper axis and improper rotation. What are the different kinds of operations generated by Sn (n = odd and even) operation?
9. Identify the quantum numbers n, l and m for the hydrogenic orbital (in a.u)

   $\psi = (\sqrt{2}/81\sqrt{\pi}) Z^{5/2} (6-Zr) Zr \exp(-Zr/3) \cos\theta$.
10. Depict the symmetry elements present in the molecules a) pyramidal NH_3 b) planar BH_3 and then identify their point groups.
11. What group is obtained by adding to or deleting from each of the following groups the indicated symmetry operations:
    a) T_d plus i b) S_6 minus i c) C_3 plus S_6 d) C_{5v} plus σ_h
12. Prove that all irreducible representations of Abelian groups must be one dimensional.
13. Define a mathematical group and a Class of the group.

(2 × 10 = 20)

SECTION B

(Answer any **5** questions. Each question carries **5** marks)

14. What is the expectation value of the momentum, Px and Px^2 for a particle in 1-dimensional box? Comment on the result.

15. Differentiate between screw axis and glide planes. Why these are not observed in molecules?

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16. What are the rules for assigning Mulliken symbols to irreducible representations? Assign Mulliken symbols to the IRs of C_2h group given below:

E	C_2	i	σh
1	1	1	1
1	1	-1	-1
1	-1	1	-1
1	-1	-1	1

17. Write down the radial equation R(r) for H atom. Derive the general solution for R(r) when r is very large (r--> ∞) and very small (r-->0).

18. The general form of Legendre differential equation is $(1-x^2)\, y'' + 2xy' + n(n+1)y = 0$.
Show that the differential equation associated with θ variable of the hydrogen atom reduces to the Legendre's equation

$\sin\theta \frac{d}{d\theta}(\sin\theta \frac{dT}{d\theta}) + (\beta \sin^2\theta - m^2)T = 0$

when $x = \cos\theta$ and $m=0$.

19. Calculate the average linear momentum of a particle described by the wave function e^{ikx} ,

where $-\infty < x < +\infty$.

20. State the great orthogonality theorem. Explain how it is helpful in constructing the character table with an example?

21. Trans 1,2-Difluoroethylene molecule has a 2-fold rotational axis, a symmetry plane perpendicular to the rotational axis and an inversion centre.
    a. What are the number of distinct symmetry operations that can be performed on the molecule?
    b. What is the number of irreducible representations of the point group of the molecule
    c. When two H-atoms of the above molecule are also replaced by F atoms, what is the point group of the resultant molecule?

(5 × 5 = 25)

SECTION C

*(Answer any **2** questions. Each question carries **15** marks)*

22. a) Set up and solve the Schrodinger equation of motion for a SHO. Deduce the expressions for wave function and energy.
    b) Calculate the zero point energy of a particle of mass 1.7×10^{-24}g connected to a spring of force constant 1×10^{4} dynes cm^{-1}.
23. a) What are spin orbital? What are their advantages over the orbitals?
    b) How does electron spin differs from classical spinning bodies? Give a brief account of electron spin operators.
24. a) Explain in detail the construction of the character table for the group C_{3v}.
    b) Reduce the C_{3v} representation Γ_a [5 2 -1]
25. Explain how group theory enables one to construct the hybrid orbitals of molecules taking BF_3 as an example.

(15 × 2=30)

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