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

M. Sc. DEGREE END SEMESTER EXAMINATION NOVEMBER 2016

SEMESTER- 1, CHEMISTRY / PHARMACEUTICAL CHEMSITRY

COURSE: P1CHET03 / P1CPHT03; QUANTUM CHEMISTRY AND GROUP THEORY

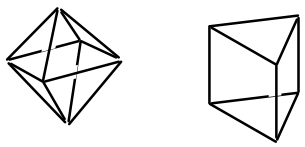
(For Supplementary / Improvement 2015 Admission)

Time: Three Hours Max. Marks: 75

Section A

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

1. What are the results of the following symmetry operations?
   a) $C_2(x)C_2(y)$ b) $\sigma(xy)\, i$ c) $\sigma(xy)\sigma(yz)$
2. What is a well-behaved function? Examine whether $y=kx^2$ is a well-behaved function. (x varies between **-∞** and **+∞**)
3. Explain the term 'degeneracy'. Give a schematic sketch of the first three energy levels obtained in a rotating particle on the surface of a ring.
4. Normallize the function sinkx and e^{ikx} in the interval x = 0 and x = 2π.
5. What is the zero point energy of Cl_2 molecule. Force constant, k=328.6 N/m.
6. Prove that the Hermitian operator always has real eigen values.
7. Set up the Schrodinger equation for hydrogen atom in spherical polar coordinates.
8. Show that $C_1e^{im\phi}$ and $C_2e^{-im\phi}$ are eigen functions of L_z operator.
9. Write down the multiplication table for C_2v point group.
10. What different point groups may the biphenyl molecule belong to depending on the rotational relationship of the two rings about the C-C bond.
11. What is transition moment operator? What is its significance?
12. Mark the different symmetry elements and thus, the point groups of the following geometries assuming equal edge lengths.



13. Write down the 3-dimensional transformation matrices for the symmetry operations
    a) reflection in xy-plane b) rotation about x-axis

(2 × 10 = 20)

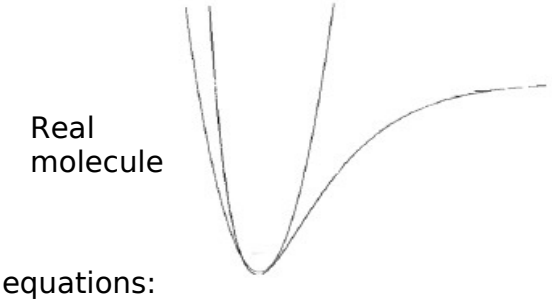
Section B

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

14. Construct the Hermite polynomial, $H_5(x)$, $a_5=2^5$.

15. Calculate the expectation value of the x-position of a particle in the state n=2 of a one-dimensional box of length a.

16. The potential energy curve for a real molecule is shown along with that for a HO



harmonic oscillator. Explain with valid equations:

(i) The origin of the differences in the two functions.

(ii) Variation of average bond length for a real molecule with vibrational energy?

17. Butadiene contains 4 π-electrons each of which moves freely from one end of the molecule to another end. Treat the molecule as one dimensional box whose length is equal to sum of all C-C bond lengths plus half the C-C bond length on either side. The average C-C bond length is 0.14nm.

a) Calculate the lowest absorption frequency in cm^{-1} and wave length in nm of light absorbed.

b) Calculate the ground state energy.

18. Briefly explain the important rules that can be deduced from Great Orthogonality Theorem.

19. a) Calculate the allowed values of polar angle θ of the orbital angular momentum vector defined by

the quantum number l=1 for an electron in hydrogen atom.

b) Write down the angular part of the orbitals d_{x2-y2} and d_{xz}.

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

21. What are eigen functions and eigen values? Provide examples of two functions which are eigen functions of both d/dx and d^2/dx^2

(5 × 5 = 25)

Section C

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

22. a) Write down the Schrodinger equation for H-atom in spherical polar coordinates and separate the

variables.

b) What is the probability of finding the electron within radius of a_0 from the nucleus? (Given ground state wave function of H-atom is $(1/\pi a_0^3)^{1/2} e^{-r/a0}$.)

23. Find out the total molecular vibrations of H_2O molecule using C_2v character table. Identify the IR and Raman activity of these vibrations.

24. Discuss the various postulates of quantum mechanics. Also explain with examples how the postulates are helpful in calculating the properties of a system.

25. a) Solve the Schrodinger equation for particle on a ring.

b) Show that the energy of the particle is quantized. What is the degeneracy of the energy levels of the particle on a ring?

(15 × 2 = 30)

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