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Name..................................

Reg. **No**..............................

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, DECEMBER 2016

(CUCSS)

Chemistry

CH 1C 01—QUANTUM CHEMISTRY AND GROUP THEORY

(2015 Admissions)

Time : Three Hours

Maximum : 36 Weightage

Part A

Answer all *questions.*
Each question carries a weightage of 1.

1. An electron is confined to one-dimensional box of length 10 nm. Find the uncertainty in momentum.
2. Which of the following are well behaved functions ? Justify your answer :

   (a) e^x **(b)** e^{ix}.

   (c) e^{-ax^2}. **(d)** Sin^{-1}

3. **How does the concept of degeneracy arise in quantum mechanical problems ?**
4. **Write Hamiltonian for (a) H_e ; (b) H_2.**
5. **Write Rodrigue's formula. Explain.**
6. **Where do you find maximum electron density for is wave function ? Justify your answer.**
7. **Explain spin functions and spin operators.**
8. **Write the examples for spherical harmonics.**
9. **Assign Schoenflies symbol of point group for the following :**

   (a) Cyclohexane (boat form).

   (b) Allene.

10. Distinguish between inverse and conjugate operations with examples.
11. Explain the term 'Gamma cart'.
12. List symmetry operations possible as D_3h. Classify them into different classes of operations.

(12 x 1 = **12** weightage)

Turn over

Part B

Answer any eight *questions.*
Each question carries a weightage of 2.

13. Show that if the operators commute they will have the same set of eigen functions and eigen values.

14. Show that $\hat{L}^2$ commutes with L_z

15. Find the average value of position of a particle confined to one-dimensional box of length a $\psi_x = \sqrt{2/a}\,\sin\left(\pi/a\right)x.$

16. Apply Schrödinger wave equation for a planar rotor. Find eigen functions and eigen values.

17. The is wave function is given as $\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$. Show that the maximum probability of find the electron is at $r = a_0$.

18. Draw polar diagrams for 3d atomic orbitals. Discuss.

19. State and explain expectation value postulate.

20. What is block diagonalization ? Explain its significance.

21. Use Great Orthogonality theorem to show that 'sum of the squares of the characters of any representation is the order of the group'.

22. Derive C_3 character table.

23. Taking the positional co-ordinates of all the atoms in ethylene $(D_{2}h)$ derive a reducible representation (write only characters of the corresponding matrices). The symmetry operations are :

    E, C2, C2, C2, σ_h, σ_v, i.

24. Generate group multiplication table for $C_{3}v$

(8 x 2 = 16 weightage)

Part C

Answer any two questions.
Each question carries a weightage of 4.

25. Apply Schrödinger wave equation for a simple harmonic oscillator. Find eigen functions and eigen values.

26. Write Great Orthogonality theorem. What are the consequences of the theorem ? Use the theorem to derive reduction formula.

27. Discuss the systematic procedure to assign Schoenflies symbol of point group.

28. Discuss briefly :

    (a) Ladder operator.

    (b) Lagendre polynomials.

    (c) Postulate of spin by Uhlenbeck and Goudsmith.

(2 x 4 = 8 weightage)