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Name...

Reg. No

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, DECEMBER 2015

(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. Calculate the de Broglie wave length of an electron accelerated by a potential of 10,000 V.

2. Write L_z in terms :

   (a) Cartesian co-ordinates.

   (b) Spherical polar co-ordinates.

3. Write recursion formula. Explain its significance.

4. Explain quantum mechanical tunneling.

5. Define spherical harmonics. Write one example.

6. Draw polar plots for 2s wave function. Explain.

7. Define spin orbital. Write one example.

8. is wave function of H atom is given as $\left(1/a\right)^{3/2} \;_{\pi}\; e^{\;.\,a.}$ Draw the wave function. Explain the nature of the plot.

9. Write Schoenflies symbol of point group for :

   (a) Cyclohexane in the chair form.

   (b) Dichloromethane.

Turn over

10. Write matrices for :

(a) C3.

(b) S3.

11. Distinguish between degenerate and non-degenerate representation with examples.

12. Find the similarity transform of any one of the vertical planes of ammonia.

(12 x 1 = 12 weightage)

Part B

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

13. Write kinetic energy operator. Show that it is a Hermitian operator.

14. Find the commutator of L_x and $\hat{L}_y$.

15. An electron is confined to a cubical box of length 10 nm. Find the wave length of the radiation required for a transition from the ground state to the first excited state.

16. Apply Schrödinger wave equation for one dimentional simple harmonic oscillator transform it into a hermite equation.

17. 2s wave function is given as $\frac{1}{4\sqrt{2\pi}}\left(\frac{1}{\ }\right)^{3/2}(2-a)\,e^{-}$. Find the value of r at which maximum probability for finding the electron is observed.

18. Using great orthogonality theorem, derive reduction formula.

19. Show that the symmetry operations E, $e_{Z(z)}$, i and σ_{xy} form a mathematical group under multiplication.

20. Taking the positional co-ordination of all atoms of cis-butadiene ($C_{2}v$). generate a reducible representation (write only characters of the corresponding matrices).

21. Using great orthogonality theorem derive C_4v character table.

22. Define Hermitian operator. Show that Hermitian operators always have real eigen values.

23. Briefly explain "space quantization".

24. Generate group multiplication table for C_3v.

(8 x 2 = 16 weightage)

Part C

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

25. **What are the postulates of quantum mechanics ? Discuss.**

26. **Apply Schrödinger wave equation for a rigid rotor. Find eigen functions and eigen values.**

27. **Apply Schrodinger wave equation for H atom. Transform into spherical polar co-ordinates. Separate the variables r, 0 and 4). Solve the Φ (phi) equation.**

28. **Discuss briefly :**

    (a) **Symmetry breaking.**

    (b) **Rodrigue's formula.**

    (c) **Dirac's relativistic equation.**

    (d) **Similarity transformation.**

(2 x 4 = 8 weightage)