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Reg. No...............................

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M.Sc. DEGREE (C.S.S.) EXAMINATION, OCTOBER 2019

First Semester

Faculty of Science

AN IC 03/AP IC 03/CH IC 03/PH IC 03/POH IC 03—QUANTUM CHEMISTRY AND
GROUP THEORY

(Common to all Branches of Chemistry)

[2012—2018 Admissions]

Time : Three Hours

Maximum Weight : 30

Section A

Answer any **ten** *questions.*
Each question carries a weight of 1.

1. Given below are Criterion functions. State which of them are eigen functions of $\dfrac{d^2}{dx^2}$. If so give the eigen values.

    (a) $A + B \sin ax$.

    (b) $A \cdot e^{ax^2}$.

2. Define Degeneracy.

3. Explain the term spherical harmonics. Write two example.

4. What are Hermite Polynomials ? Give one example.

5. Draw the radial distribution function for $2s$, $2p$ and $3s$ orbitals ?

6. What are the characteristic operations of an s_6 axis ? Construct their matrix representation in the basic (x, y, z).

7. Write down the character of the reducible representation of composition :

    $\Gamma = A_1 + A_2 + B_1 + B_2$ of the C_{2V} group.

8. Generate matrices for s_3 and i.

9. What is meant by optical activity ? What are the criterion for it ?

10. What are the selection rules for the vibrational absorption of a molecule ?

Turn over

11. Explain the term pre-dissociation.

12. What are the internal standards used in ESR spectroscopy ?

13. In what respects the quantum mechanical harmonic oscillator differs from classical oscillator ?

$(10 \times 1 = 10)$

Section B

Answer any **five** *questions.*
Each question carries a weight of 2.

14. Show that the eigen functions corresponding to different eigen values of a Hermitian operator are always orthogonal.

15. Compare the Cartesian and spherical polar co-ordinates.

16. Evaluate the commutators $\left[\hat{x}\, \hat{P}r \right]$ and $\left[\hat{L}_x, \hat{L}_y \right]$.

17. Is wave function of H atom is $\psi = \dfrac{1}{\sqrt{\pi}} \left(\dfrac{1}{a_0} \right)^{3/2} e^{-r/a_0}$, show that maximum probability for finding the electron is at $r = a_0$.

18. Find the similarity transform and inverse of any *one* vertical plane in NH_3.

19. What is meant by block diagonalization ? Explain its importance.

20. Explain the important properties of irreducible representations.

21. Outcome the principle of ESR spectroscopy.

$(5 \times 2 = 10)$

Section C

Answer any **two** *questions.*
Each question carries a weight of 5.

22. (a) State and explain wave function postulate and expectation value postulate of quantum mechanics.

    (b) Explain the discovery of spin using an experiment.

23. Show that the normalised wave function for a particle in a 3–D box with sides of length a, b and c is $\psi(x, y, z) = \left(\dfrac{8}{abc}\right)^{1/2} \sin\left(n_x\, \pi \dfrac{x}{a}\right) \sin\left(n_y\, {}^{\pi y}\!/\!_b\right) \sin\left(n_z\, {}^{\pi z}\!/\!_c\right)$ and discuss the degeneracies of the first few energy levels.

24. (a) Set up Schrödinger wave equation for the hydrogen atom. Transform the co-ordinates and separate the variables.

    (b) Discuss briefly the origin of Raman Spectrum.

25. Apply orthogonality theorem for C_{3v} point group and derive the character table.

$(2 \times 5 = 10)$