23P110   (Pages: 2)   Name: …………………….

Reg. No……………………

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2023
(CUCSS-PG)

(Regular/Supplementary/Improvement)

CC19P CHE1 C01 – QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY
(Chemistry)

(2019 Admission onwards)

Time: Three Hours   Maximum: 30 Weightage

Section A
Answer any *eight* questions. Each question carries 1 weightage.

1. What do you mean by space quantisation? Explain.

2. Express $\hat{L}_z$ in cartesian and spherical polar coordinates.

3. State and explain postulate of spin by Goudsmit.

4. What is Ladder Operator?

5. Show that $A \sin k\, x$ and e^{ax} are eigen functions of $\frac{d^2}{dx^2}$. Find the corresponding eigen values.

6. Explain the spherical harmonics of s orbital.

7. What is GTO? Write one example.

8. Write the Slater determinant for Li atom.

9. What is meant by force field in molecular mechanics?

10. Construct the Z-matrix of CH_3OH.

11. What is density functional theory?

12. Discuss Roothan's concept of basis functions.

(8 × 1 = 8 Weightage)

Section B
Answer any *four* questions. Each question carries 3 weightage.

13. Explain concept of perturbation method using particle in one dimensional box with slanted bottom.

14. Find the eigen functions and eigen values for 'particle in a ring problem'.

15. Derive radial distribution function.

16. Discuss the features of 'particle in a rectangular well' system.

17. Define Hermitian operator. Prove that the Hermitian operators have real eigen values.

18. Construct the Z-matrix of HCHO & NH_3.

19. Discuss the classification of computational chemistry methods.

(4 × 3 = 12 Weightage)

Section C

Answer any *two* questions. Each question carries 5 weightage.

20. Apply Schrodinger wave equation for one dimensional SHO. Find eigen functions and eigen values.

21. Solve R- equation of H atom.

22. Explain Hartree's Self-Consistent Field method for atoms in quantum mechanics.

23. Discuss the classification of basis sets used in computational chemistry calculations.

(2 × 5 = 10 Weightage)

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