22P110 (Pages: 2) Name: ……………………

Reg. No……………………

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2022

(CBCSS-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. Which of the functions are eigen functions of operator; d^2/dx^2?

   (a) Sin5x (b) 8cos2x (c) $4x^2$
2. Write recursion formula. Explain its significance.
3. Explain 'quantum mechanical tunneling'.
4. Define Spin-Orbital. Write one example.
5. An electron is confined to a cubical box of length 10 nm. Find the ground state energy.
6. Write Rodrigue's formula. Explain its significance.
7. Write the Slater determinant for Li atom.
8. What is a radial distribution function? Sketch the radial distribution function of 2s and 2p atomic orbitals.
9. Discuss the need of post-HF methods in computational calculations.
10. Distinguish between Slater type and Gaussian type orbitals.
11. What are electronic structure methods?
12. What is meant by a force field?

(8 × 1 = 8 Weightage)

Section B

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

13. Explain concept of peturbation method using particle in one dimensional box with slanted bottom.
14. Define Hermitian operator. Prove that the Hermitian operators have real eigen values.
15. Define the term degeneracy of an energy level. Calculate the degeneracies of a particle in a 3D cubical box having energies equal to i) 6 and ii) 14 in units of $h^2/8ma^2$.
16. Solve Θ equation to derive the wave function and energy for a non-planar rigid rotator.
17. Solve He atom using variation method.

18. Show that $\hat{L}^2$ and $\hat{L}_z$ commute.

19. Construct the Z-matrix of CH_3OH and NH_3 molecules.

(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. Explain Hartree-Fock SCF method for solving many electron atoms, quantum mechanically.

22. Apply Schrodinger wave equation for H atom. Transform into spherical polar coordinates. Separate the variables and solve the R equation.

23. Define basis set. Write notes on different types of basis sets used in computational chemistry calculations.

(2 × 5 = 10 Weightage)

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