24P110 (Pages: 2) Name: ….……

Reg. No……

FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2024

(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. Show that the momentum operator is Hermitian.
2. What is a conservative system?
3. Write the recursion formula. Explain its significance.
4. Express $\hat{L}_z$ in Cartesian and spherical polar coordinates.
5. Define Spin-Orbital.
6. State and explain variation theorem.
7. What is GTO? Write one example.
8. Write the Slater determinant for Li atom.
9. Define Fock operator.
10. How does 'degeneracy' arise in quantum mechanical problems?
11. Explain the term force field. Give two examples.
12. What is radial distribution function?

(8 × 1 = 8 Weightage)

Section B

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

13. Explain quantum mechanical tunneling.
14. Briefly discuss the postulates of quantum mechanics.
15. Find the commutator of $\hat{L}^2$and $\hat{L}_z$.
16. Derive first Bohr radius of H atom.
17. Explain concept of perturbation method using particle in a one-dimensional box with slanted bottom.
18. Solve *He*-atom using variation method.
19. Find the eigen functions and eigen values for 'particle in a ring problem'.

(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-Fock Self-Consistent Field method.
23. What is Z-matrix of a molecular geometry? Construct the Z-matrix of (i) H_2O (ii) CH_3OH and (iii) HCHO molecules.

(2 × 5 = 10 Weightage)

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