FIRST SEMESTER M.Sc. DEGREE EXAMINATION, NOVEMBER 2020
(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. What do you mean by a conservative system?

2. Write the time dependent Schrödinger wave equation.

3. What is the many body problem faced in quantum mechanics?

4. Write the spin orbital for $1s^2$ configuration.

5. Write recursion formula. Explain the significance.

6. Give an example of a Pople-style basis set.

7. What is a radial distribution function? Sketch the radial distribution function of 3s and 2p atomic orbitals.

8. What is meant my quantum mechanical tunneling?

9. Write the Slater determinant for Li atom. Show that the maximum occupancy of an orbital is 2.

10. What is STO? Write one example.

(8 x 1 = 8 Weightage)

Section B
Answer any *six* questions. Each question carries 2 weightage.

11. Explain Pauli's anti symmetry principle.

12. Write Z-matrix for ammonia using internal coordinates.

13. For simple harmonic oscillator deduce the expression for wave function ψ_0 and ψ_1 using hermite polynomial solution.

14. Define the term degeneracy of an energy level. Calculate the energies of doubly and triply degenerate states.

15. For diatomic Simple harmonic oscillators, find the expectation value of kinetic energy operator if the system is in first energy level and show that it is Hermitian.

16. Enunciate the modifications made by Fock in Hartree -Fock theory and brief limitations of Hartree -Fock method.

17. Show that $Lx^\wedge$ and $Ly^\wedge$ do not commute.

18. Apply Schrodinger wave equation for H atom. Transform it into spherical polar co-ordinates. Separate the variables r, Θ, φ.

(6 x 2 = 12 Weightage)

Section C

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

19. Apply Schrödinger equation for rigid rotor. Find Eigen functions and Eigen values.

20. Setup the Schrödinger equation for hydrogen atom and separate the variables to obtain R, Θ and Φ equations. Write the general solution of these equations.

21. What do you mean by first order perturbation methods? Determine the ground state energy of a particle in one dimensional box with slanted bottom using perturbation method.

22. Explain in detail the Hartree-Fock Self-consistent field method for atoms.

(2 x 5 =10 Weightage)

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