

D 32671

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Name.....

Reg. No.....

FIRST SEMESTER M.Sc. (CBCSS) REGULAR/SUPPLEMENTARY DEGREE
EXAMINATION, NOVEMBER 2022

Chemistry

CHE1C01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admission onwards)

Time : Three Hours

Maximum Weightage : 30

Section A

Answer any **eight** questions.

Each question carries a weightage of 1.

- Which of the following one well behaved functions :
(a) e^x ; (b) e^{ix} ; (c) e^{-ax^2} ; (d) $\sin^{-1} x$.
- Explain with example 'conservative system'.
- The energy of a particle in cubical box of length 'a' is $\frac{14h^2}{8ma^2}$. What is the degeneracy of the level.
- Explain the term 'Symmetry breaking'.
- The solutions of a planar rotor are $\frac{1}{\sqrt{\pi}} e^{im\phi}$. Express it as a real function.
- 1s wave function for H atom is Ae^{-r/a_0} . Represent the function graphically. Explain.
- State and explain independent particle model.
- What do you mean by 'Slater type of orbitals' ? Write one example.
- Explain the term 'molecular mechanics' in computational chemistry.
- Write Z-matrix for NH_3 .

(8 × 1 = 8)

Section B

Answer any **six** questions.

Each question carries a weightage of 2.

- Show that eigen functions of a Hermitian operator are mutually orthogonal.

Turn over

12. Write Rogrigue's formula. Use the formulate to find $H_{(X)}$ for $\nu = 4$ in simple harmonic oscillator.
13. Find the commutator of \hat{L}_x and \hat{L}_y .
14. 1s wave function for H atom is Ae^{-r/a_0} . Show that the maximum probability of finding the electron is at $r = a_0$.
15. State and prove Variation theorem.
16. Briefly discuss Fock's modification of Hartree self consistent field method.
17. Compare semi empirical and abinitio methods of computational chemistry.
18. How do you classify basis sets ? Discuss.

(6 × 2 = 12)

Section C

Answer any two questions.

Each question carries a weightage of 5.

19. Discuss postulates of quantum mechanics.
20. Apply Schrödinger wave equation for a spherical rotor. Find eigen functions and eigen values.
21. Use variation theorem to find the ground state energy of particle in one dimensional box with slanted bottom.
22. (a) Find the ground state energy of He by first order Perturbation method.
(b) What are the general features of a Gaussian input file ? Discuss.

(2 × 5 = 10)