**32671** (Pages : 2) 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 weightate of 1.*

1. Which of the following one well behaved functions :

    (a) $e^x$; (b) $e^{ix}$; (c) $e^{-ax^2}$; (d) $\sin^{-1} x$.

2. Explain with example 'conservative system'.

3. The energy of a particle in cubical box of length 'a' is $\dfrac{14h^2}{8ma^2}$. What is the degeneracy of the level.

4. Explain the term 'Symmetry breaking'.

5. The solutions of a planar rotor are $\dfrac{1}{\sqrt{\Pi}} e^{im\phi}$. Express it as a real function.

6. 1s wave function for H atom is $Ae^{-r/a_0}$. Represent the function graphically. Explain.

7. State and explain independent particle model.

8. What do you mean by 'Slater type of orbitals' ? Write one example.

9. Explain the term 'molecular mechanics' in computational chemistry.

10. Write Z-matrix for $NH_3$.

                                                            $(8 \times 1 = 8)$

## Section B

*Answer any* **six** *questions.*
*Each question carries a weightage of 2.*

11. 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 $v = 4$ in simple oscillator.

13. Find the commutator of $\hat{L}_x$ and $\hat{L}_y$.

14. Is wave function for H atom is $Ae^{-r/a_0}$. Show that the maximum probability of fin 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.

## 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 a values.

1. Use variation theorem to find the ground state energy of particle in one dimens with slanted bottom.

2. (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.