

FIRST SEMESTER M.A./M.Sc./M.Com. DEGREE EXAMINATION  
DECEMBER 2019

(CBCSS)

Chemistry

CHE 1C 01—QUANTUM MECHANICS AND COMPUTATIONAL CHEMISTRY

(2019 Admissions)

Time : Three Hours

Maximum : 30 Weightage

**Section A**

*Answer any eight questions.*

*Each question carries 1 weightage.*

- Which of the following are well behaved functions ? Justify your answer :
  - $\sin^{-1} x$ .
  - $e^{ix}$ .
  - $e^{x^2}$ .
  - $e^{-x}$ .
- Find the commutator of  $x$  and  $\frac{d}{dx}$ .
- The energy of a particle in a cubical box of length 'l' is  $\frac{14h^2}{8ml^2}$ . Find the degeneracy.
- Write recursion formula. Explain its significance.
- Define spherical harmonics.
- The 1s wave function for H atom is  $\psi_{1s} = Ne^{-r/a_0}$ . Plot the function against  $r$ . Explain the significance.
- State and explain 'independent particle model'.
- Explain with example STO.
- With the help of one example explain 'Molecular Mechanics' method.
- What is split valence basis set ?

(8 × 1 = 8 weightage)

**Section B**

*Answer any six questions.*

*Each question carries 2 weightage.*

- Show that if two operators commute they will have the same set of eigen functions and eigen values.

Turn over

12. Use particle in one dimensional box model to understand quantum mechanical tunneling.
13. Show that  $\hat{L}^2$  commutes with  $\hat{L}_z$ .
14. Discuss the shapes of the following orbitals (a)  $N(3\cos^2\theta - 1)$  (b)  $N\sin\theta\cos\theta$ .
15. State and prove variation theorem.
16. Briefly discuss HF self consistent field method.
17. Compare *ab-initio* and semi empirical method of computational chemistry.
18. Discuss the structure of a Gaussian in put file.

(6 × 2 = 12 weightage)

### Section C

*Answer any two questions.*

*Each question carries 5 weightage.*

19. Discuss postulates of quantum mechanics.
20. Apply schrödinger wave equation for a simple harmonic oscillator. Find eigen functions and eigen values.
21. Apply schrödinger wave equation for H atom. Transform into spherical polar co-ordinates. Separate the variables. Solve the  $\Phi(\phi)$  equation.
22. Use perturbation method to find the ground state energy of a particle in one dimensional box with slanted bottom.

(2 × 5 = 10 weightage)