

CHE 502

M.Sc. (Ist Semester) EXAMINATION, 2023-24

(CBCS Mode)

CHEMISTRY

(Quantum Chemistry-I)

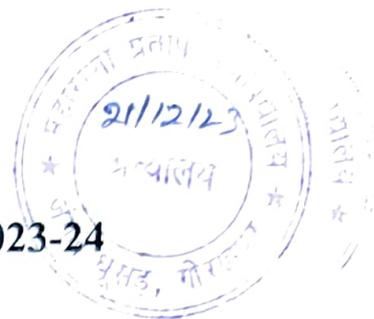
Time : Three Hours]

[Maximum Marks : 75

Note: There are **three** sections (A, B and C) and Candidate has to attempt questions from all **sections**. Marks are indicated against each section.

Section-A

1. Answer all question. 5×3=15
- (a) What do you mean by Linear operator ?
 - (b) Why approximate methods are needed for solving Schrodinger wave equation for multi electron atoms ?
 - (c) What are the necessary conditions for the application of perturbation theory ?
 - (d) What are Hermitian operators ?
 - (e) What do you mean by rigid rotor ?



Section-B

Note: Answer all question of the following. $4 \times 5 = 20$

2. (a) What is simple harmonic motion (S.H.M.) ?
Discuss the energy levels of Harmonic and An-harmonic oscillators.

Or

- (b) Describe Hartree self-consistent field method for the solution of wave function of a many electron system.
3. (a) Discuss the principle of variation method in quantum mechanical calculations with the help of one example.

Or

- (b) For the Hermitian operator, prove that-
- (i) Eigen values are real
 - (ii) Eigen functions corresponding to different Eigen values are orthogonal to each other.
4. (a) Explain quantum mechanical treatment of Harmonic oscillator.

Or

- (b) Discuss the application of perturbation theory for the calculation of ground state energy of He atom.

5. (a) Explain Postulates of Quantum mechanics.

Or

- (b) Derive the expression for the energy levels of a three dimensional rigid rotor.

Section-C

Note: Answer any two questions of the following. $2 \times 20 = 40$

6. Derive the expression for energy and wave function for a micro particle moving in a three dimensional box. Describe the concept of degeneracy of states.
7. Write the Schrodinger wave equation for H atom in polar coordinates. Separate the variables and solve the ϕ part of the equation.
8. Obtain expression for the first order perturbation corrections to the energy and wave function of the unperturbed system.
9. What are acceptable wave function ? Discuss the condition for normalisation and orthogonality in wave function. derive Schrodinger wave equation.

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