CHE 502

M.Sc. (I[st] Semester) EXAMINATION, 2023-24

(CBCS Mode)

CHEMISTRY

(Quantum Chemistry-I)

1384

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. 2×20=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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