

BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI  
(END SEMESTER EXAMINATION)

CLASS: M.SC.  
BRANCH: CHEMISTRY

SEMESTER : II  
SESSION : SP/19

SUBJECT: CH409 QUANTUM CHEMISTRY & GROUP THEORY

TIME: 3 Hours

FULL MARKS: 50

**INSTRUCTIONS:**

1. The question paper contains 5 questions each of 10 marks and total 50 marks.
  2. Attempt all questions.
  3. The missing data, if any, may be assumed suitably.
  4. Before attempting the question paper, be sure that you have got the correct question paper.
  5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.
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- Q.1(a) Derive the Hamiltonian operator for a particle of mass  $m$ . [5]
- Q.1(b) Calculate the energies and wave functions for a particle in an infinite one-dimensional box, with potential energy zero inside the box. What will happen if the walls of the one-dimensional box are suddenly removed? [5]
- Q.2(a) For a particle in the states  $n = 1$ , and  $3$  of a one-dimensional box of length  $L$ , find the probability that the particle is in the region  $0 \leq x \leq L/4$  [5]
- Q.2(b) Discuss the solution of Schrödinger wave equation for a particle in three-dimensional cubic box with edges of length 'a' assuming that the potential is zero within the box and infinite outside the box. What is meant by degeneracy of energy levels? [5]
- Q.3(a) The vibrational energy levels of simple harmonic oscillator are given as  $E_n = (n + \frac{1}{2}) h\nu$ . Sketch the first four energy levels and find the difference between them. [5]
- Q.3(b) Compare the result of classical and quantum mechanical treatment of simple harmonic oscillator. [5]
- Q.4(a) What is Hartree-Fock self-consistent field theory? [5]
- Q.4(b) Determine the term symbol for a  $p^3$  configuration of nitrogen atom. Arrange the different state in order of increasing energy. How many micro-states exist for this configuration? [5]
- Q.5(a) Form the irreducible representations for  $C_{2v}$  point group using translational vectors as basis of representation. Assign Mulliken symbols with each representation. [5]
- Q.5(b) What is great orthogonality theorem? Prove it with respect to irreducible representations deduced for  $C_{2v}$  point group. [5]

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