

End Semester Examinations - 2015-16 Even Semester - May 2016

15CH3004 Quantum Chemistry and Group Theory

Set B

Time : 3 hrs
Total Marks: 100

1. 1.a. What is Compton effect? Explain with a diagram. (5 marks)
1.b. Describe the postulates of quantum mechanics (5 marks)
1.c. Derive Schrodinger wave equation. Describe the significance of wave function. (10 marks)

OR
2. 2.a. Derive the equations for energy and normalized wave function for the particle in one-dimensional box. (10 marks)
2.b. Describe the theory of simple harmonic oscillator. (10 marks)
3. 3.a. Describe time-dependent perturbation theory (10 marks)
3.b. What is variation theorem? Derive its proof. (10 marks)

OR
4. 4.a. Derive the determinant form of the wave function of a many electron system. (10 marks)
4.b. Describe the theory of Born Oppenheimer approximation. (10 marks)
5. 5.a. Describe the molecular orbital (MO) treatment of hydrogen molecule. (10 marks)
5.b. Describe the Simple Hückel theory for the cyclic conjugated systems. (10 marks)

OR
6. 6.a. What is a proper axis of symmetry? Explain whether the proper axis of symmetry is present in the following molecules having different geometries: (i) AB₂ (Bent); (ii) AB₃ (Planar); (iii) AB₄ (Square Planar); (iv) AB₄ (Tetrahedral); (v) AB₅ (Pentagonal). (10 marks)
6.b. What is a group multiplication table? What is its importance? Draw the group multiplication tables for C_{2v} and C_{3v} point groups. (10 marks)
7. 7.a. What are conjugate elements? Explain with few examples. (10 marks)
7.b. State the important postulates of Great Orthogonality Theorem (GOT)? Construct the character table for C_{3v} point group using GOT? (10 marks)

OR
8. 8.a. What is direct product group? Explain with few examples. (10 marks)
8.b. How will you determine the irreducible representations of the vibrational modes present in water molecule. Explain the procedure. (10 marks)
9. 9.a. Correlate the symmetry of molecular orbitals and electronic states of formaldehyde (10 marks)
9.b. Explain the hybridization schemes present in water molecule using group theory (10 marks)