Reg.No. \_\_\_\_\_\_\_\_\_\_\_\_



**UNIVERSITY**

(Karunya Institute of Technology & Sciences)

(Declared as Deemed-to-be University under Sec.3 of the UGC Act, 1956)

**Supplementary Examination – June – 2017**

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| **Code :** | **15CH3004** | **Duration :** | **3hrs** |
| **Sub. Name :** | **QUANTUM CHEMISTRY AND GROUP THEORY** | **Max. marks :** | **100** |

**ANSWER ALL QUESTIONS (5 x 20 = 100 Marks)**

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| Q. No. | Sub Div. | Questions | Course  Outcome | Marks |
| 1. | a. | Derive de Broglie equation. Find out the de Broglie wave length of a tennis ball of mass 0.050 kg and moving at a velocity of 20m/s . | CO5 | 10 |
| b. | Write a short note on the following. a) Work function b) Wave particle duality c) Normalization of wave function d) Operator d) Hamiltonian operator. | CO2 | 10 |
| (OR) | | | | |
| 2. | a. | Solve the Schrodinger equation for Hydrogen atom. Using the Radial plots and angular plots for hydrogen atom, predict the size and shape of the atomic orbital. | CO2 | 15 |
| b. | Define Zero point energy. What will be the zero point energy in Harmonic oscillator and rigid rotor? | CO2 | 5 |
| 3. | a. | Calculate the energy of H2+ molecule using Molecular Orbital Theory | CO3 | 15 |
|  | b. | Find out the four quantum numbers for the two electrons present in 5S orbital. Prove Pauli’s statement. | CO3 | 5 |
| (OR) | | | | |
| 4. | a. | Explain the following terms  a) Variation theorem b) Born Oppenheimer approximation  c) Hamiltonian of H2 molecule | CO1 | 10 |
|  | b. | Describe Huckels theory for the molecular orbitals (HMO) of Allyl cation | CO3 | 10 |
| 5. | a. | State Aufbau Principle and Hund’s rule of maximum multiplicity. Apply them to find out the electronic configuration of atom with atomic number 12 and 25. | CO3 | 10 |
|  | b. | Explain your understanding about Rigid Rotar. What will be the energy of rigid rotor? | CO2 | 10 |
| (OR) | | | | |
| 6. | a. | Discuss on the salient features of character table. Explain with the Character table of C2V point group. | CO4 | 12 |
|  | b. | Predict the point group of Ammonia. What will be the point group if σh is introduced to the ammonia molecule? | CO5 | 4 |
|  | c. | Give one example each for D3d and D3h point group symmetry. Discuss the symmetry elements present in the molecule | CO4 | 4 |
| 7. | a. | Find out the irreducible representation for the X, Y, Z coordinates and the rotational axis along X, Y and Z directions for water molecule. | CO3 | 6 |
|  | b. | Show the various axis of symmetry (C) in the octahedral and tetrahedral shapes. | CO4 | 4 |
|  | c. | Define the following terms with suitable example a) Inversion centre b) Dimension of IRR c) Order of the group d) t2g and eg e) Laporte selection rule. | CO2 | 10 |
| (OR) | | | | |
| 8. | a. | Predict the shape, symmetry elements and the point group symmetry for the following molecules. i) Ammonia ii) water iii) ICl5 iv) [PtCl4]2- | CO3 | 12 |
|  | b. | Predict the irreducible representation for the vibrational modes of water molecule. | CO3 | 8 |
|  | | **Compulsory**: |  |  |
| 9. | a. | Discuss on the reduction formula for decomposing reducible representation to irreducible representation taking C2V character table as example. | CO5 | 12 |
|  | b. | Predict the structure of BCl3 after carrying out the following successive operations.  a) C2C3E  b) C3EC2 | CO3 | 8 |

ALL THE BEST