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



**UNIVERSITY**

(Karunya Institute of Technology & Sciences)

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

**End Semester Examination – April/May – 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. | Solve the Schrödinger equation for a particle confined in a one dimensional box. Calculate the energy, momentum and normalization parameter? | CO2 | 12 |
| b. | Define Eigen function and Eigen value. Prove that AsinnΠx/λ is an Eigen function of the operator d2/dx2. What will be the Eigen value? | CO5 | 8 |
| (OR) | | | | |
| 2. | a. | Write a short note on Photoelectric effect. | CO1 | 8 |
| b. | The work function for metallic cesium is 3.43 x 10-19 J. Calculate the kinetic energy of the electrons ejected by light of 300 nm wavelength. [*Given:* Planck's constant = 6.626 x 10-34 J s; the speed of light = 3.00 x 108 m/s] | CO5 | 6 |
| c. | How will you convert the Cartesian coordinate into spherical coordinate? | CO2 | 6 |
| 3. | a. | Derive Schrödinger equation. What are the significances of Schrodinger Equation. | CO1 | 10 |
|  | b. | Write a short note on a) Black body radiation b) Hydrogen spectrum. | CO1 | 10 |
| (OR) | | | | |
| 4. | a. | Derive the first order and second order correction terms in perturbation theory. | CO2 | 10 |
|  | b. | What are the postulates of Molecular orbital theory? | CO1 | 6 |
|  | c. | Write a short note on Anti-symmetry principle and Slater determinant. | CO2 | 4 |
| 5. | a. | Discuss on the theory of hybridization. What is the hybridization of Sulphur in SF6 and SF4 | CO3 | 8 |
|  | b. | Discribe the HMO theory for butadiene. Calculate the energy levels of HMO’s and give the physical representation of them. | CO2 | 12 |
| (OR) | | | | |
| 6. | a. | Write a short note on the various symmetry elements and their operations with suitable examples. | CO2 | 12 |
|  | b. | Predict the symmetry (gerade and ungerade) in the bonding and anti bonding molecular orbitals of S, Pz, Px. | CO4 | 8 |
| 7. | a. | Define the following terms a) Abelian group b) Associative property c) Commutative property d) Gerade and ungerade e) Mutual exclusion principle. | CO2 | 10 |
|  | b. | Explain Great orthogonality theorem with suitable example. | CO2 | 10 |
| (OR) | | | | |
| 8. | a. | Predict the structure of the molecule after carrying out the following successive operations.   1. Eσxyσyz in water molecule 2. C3EC2 in BCl3 molecule | CO3 | 10 |
|  | b. | Give the character table of water molecule. What are the terms we use in charater table and what do they mean? | CO2 | 10 |
|  | | **Compulsory:** |  |  |
| 9. | a. | Predict the shape, symmetry elements and the point group symmetry for the following molecules. i)CO2 ii) PCl5 iii) BF3 iv) XeOF4 | CO3 | 10 |
|  | b. | Give the MO’s of ethylene and butadiene. Mention the symmetry of MO’s with respect to axis of symmetry and plane of symmetry. | CO3 | 10 |

ALL THE BEST