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



**End Semester Examination – Nov/Dec – 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. | Calculate the energy, momentum and normalization parameter for a particle confined in a one dimensional box using Schrodinger equation. | CO3 | 12 |
| b. | Define the following terms i. Eigen function ii. Eigen Value  iii. operator iv. Angular momentum. | CO2 | 8 |
| (OR) | | | | |
| 2. | a. | Write a short note on hydrogen spectrum. | CO1 | 8 |
| b. | The velocity of a ball bowled by Kapli Dev is 25 km/sec. Calculate the wavelength of the matter wave associated with the ball. (Mass of the cricket ball is 0.1585kg, h=6.626 x10-34 m2kg/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 ψ and ψ2. | CO1 | 15 |
|  | b. | Write a short note on Black body radiation. | CO1 | 5 |
| (OR) | | | | |
| 4. | a. | Derive the first order and second order correction terms in perturbation theory. | CO2 | 14 |
|  | b. | Write a short note on Anti-symmetry principle. | CO1 | 6 |
|  |  |  |  |  |
| 5. | a | Discuss on the theory of hybridization. What is the hybridization of Nitrogen in Ammonia? | CO3 | 8 |
|  | b | Calculate the energy levels of Huckel’s Molecular Orbitals of butadiene and give the physical representation of them. | CO2 | 12 |
| (OR) | | | | |
| 6. | a. | Discuss on the following symmetry elements with suitable example  i. Principle axis of symmetry ii. Inversion center iii. σh and σv | CO3 | 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  i. Mutual exclusion principle ii. Mulliken symbol iii. Raman active and IR active vibrational mode iv. g and u in character table. | CO2 | 10 |
|  | b. | Explain Great orthogonality theorem taking C3V point group as example.   |  |  |  |  | | --- | --- | --- | --- | | C3V | E | 2C3 | 3σv | | A1 | 1 | 1 | 1 | | A2 | 1 | 1 | -1 | | E | 2 | -1 | 0 | | CO2 | 10 |
| (OR) | | | | |
|  |  |  |  |  |
| 8. | a. | Predict the structure of the molecule after carrying out the following successive operations.   1. C2σyzC2 in water molecule 2. C3S3C2 in PCl5 molecule | CO3 | 10 |
|  | b. | Give the character table of C2V point group. Explain the terms and symbols we use in the character table. | CO2 | 10 |
|  | |  |  |  |
|  | | **Compulsory**: |  |  |
| 9. | a. | Predict the shape, symmetry elements and the point group symmetry for the following molecules. i. Benzene ii. BCl3 iii. CH4 iv. XeF4. | CO4 | 10 |
|  | b. | Give all the vibrational modes of water molecule. Predict the irreducible representation for the vibrational modes. | CO4 | 10 |

ALL THE BEST