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

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**End Semester Examination –Nov / Dec – 2019**

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| **Code :** | **17CH3004** | **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. | | Describe the importance of black body radiation with a diagram. | CO1 | 10 |
| b. | | Explain the wave nature of electron with Davidson and Germer experiment. | CO1 | 10 |
| **(OR)** | | | | | | |
| 2. | | a. | | Calculate the uncertainty in position of an electron if the uncertainty in velocity is 5.7 x 105 mS-1(h = 6.6 x 10-34 Kgm2Sec-1 and mass of electron = 9.1 x 10-31 Kg) | CO1 | 5 |
| b. | | Describe the following: (i) Operator (ii) Commutator | CO1 | 5 |
| c. | | Explain the postulates of quantum mechanics. | CO1 | 10 |
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| 3. | | a. | | Describe the theory of particle in one dimensional box. | CO2 | 10 |
| b. | | Derive the expressions for the normalized wave function and rotational energy levels of rigid rotor. | CO2 | 10 |
| **(OR)** | | | | | | |
| 4. | | a. | | Derive the Schrodinger equation for hydrogen atom. | CO2 | 10 |
| b. | | Explain the principle of variation theorem and its application to the ground state of helium atom. | CO2 | 10 |
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| 5. | | a. | | Explain the theory of Slater determinantal wave functions. | CO2 | 10 |
| b. | | Describe the Simple Huckeltheory of the linear conjugated systems. | CO3 | 10 |
| **(OR)** | | | | | | |
| 6. | | a. | | Describe the linear combination of atomic orbital (LCAO) treatment of hydrogen molecule. | CO3 | 10 |
| b. | | Describe the theory of Born oppenheimer approximation. | CO2 | 10 |
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| 7. | | a. | | Explain the centre of symmetry present in the following molecular configurations. (i) AB2 (Bent); (ii) AB3 (Planar); (iii) AB3 (Pyramidal); (iv) AB4 (Square planar); (v) AB6 (Octahedral). | CO4 | 10 |
| b. | | Explain the following: (i) Order of a group; (ii) Conjugate elements and classes. | CO4 | 10 |
| **(OR)** | | | | | | |
| 8. | a. | | Describe Great Orthogonality Theorem (GOT). How do you construct the character table for the C3vpoint group using GOT? | | CO4 | 10 |
| b. | | Explain the theory of direct product groups. | | CO4 | 10 |
|  |  | | **Compulsory:** | |  |  |
| 9. | a. | | Describe the rules for determinining the irreducible representations of the vibrational modes in nonlinear molecules. | | CO5 | 10 |
| b. | | Describe the hybridization schemes for atoms in methane molecule. | | CO6 | 10 |