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



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

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| **Code :** | **17PH3034** | **Duration :** | **3hrs** |
| **Sub. Name :** | **MOLECULAR QUANTUM MECHANICS** | **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 Hartree-Fock self consistent field method. Use the method in the treatment of many electron atoms. | CO1 | 10 |
| b. | Give an account on Born-Oppenheimer approximation. Explain how it is used to separate electronic and nuclear motions in a quantum mechanical system. | CO2 | 10 |
|  | **(OR)** | | | |
| 2. |  | The one electron H2+ ion furnishes many ideas useful for discussing many-electron diatomic molecule. Using the necessary approximate treatments obtain the atomic probability densities for H2+ ground electronic state. | CO2 | 20 |
|  |  |  |  |  |
| 3. | a. | Compare and explain the molecular-orbital (MO) and valence bond (VB) treatments of the H2 ground state molecule. | CO3 | 10 |
| b. | Obtain the MO and VB wave functions for homonuclear diatomic molecules. | CO3 | 10 |
|  | **(OR)** | | | |
| 4. |  | How does the Hellmann-Feynman theorem treat many electron systems? Discuss the theory in detail. | CO3 | 20 |
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| 5. | a. | Describe in detail the theory involved in the SCF MO treatment of polyatomic molecule. | CO4 | 10 |
| b. | Write notes on the following:   1. Population analysis. 2. Dipole moment. | CO4 | 10 |
|  | **(OR)** | | | |
| 6. | a. | From the geometry of the given system how do you find their vibrational frequencies and henceforth discuss their thermodynamic properties? | CO5 | 10 |
| b. | Give an account on the thermochemical stabilities of the molecules of the geometry optimized structure. | CO5 | 10 |
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| 7. |  | Give an overview about the Thomas-Fermi model and briefly describe the Thomas-Fermi-Dirac-Weizsacker model. | CO5 | 20 |
|  | **(OR)** | | | |
| 8. |  | How does the local density approximation (LDA) of Hohenberg and Kohn vary from the generalized gradient approximation (GGA). Describe in detail. | CO5 | 20 |
|  | | **Compulsory:** |  |  |
| 9. | a. | Discuss in detail the chemical potential in the grand canonical ensemble at zero temperature along with their physical meaning. | CO6 | 10 |
| b. | Explain the theory involved in the chemical potential for a pure state and in the canonical ensemble. | CO6 | 10 |