2015

CHEMISTRY

Paper : 301

QUANTUM CHEMISTRY

Full Marks : 80

Time : 3 hours

The figures in the margin indicate full marks for the questions

1. Write down the Hamiltonian for anharmonic oscillator and identify the perturbed term. 2

2. Describe the perturbation method to calculate the first order correction term for the Eigen function. 4

3. Discuss the application of perturbation treatment to the ground state of *He* atom. 7

4. Briefly discuss about the Variation method. What are steps involved in applying variation method to a system? 4+3 =7

5. How many roots of $\overline{E}$ are possible for a secular determinant of k^{th} order? 1

6. Calculate the energy for excited states of *He* using variation method. 9

7. Write down the trial wave function for H_2^+ in LCAO-MO framework. 1

8. Discuss the VB treatment of hydrogen molecule. 9

9. Compare MO treatment with VB treatment for H_2 molecule. 5

10. Discuss the LCAO-MO treatment of H_2O. 7

11. Discuss the application of Huckel approximation to conjugated organic molecules. 4

12. In polyene system, red shift is observed for $\pi \rightarrow \pi^*$ transition with incorporation of more and more conjugation to the system. Why? Explain. 4

13. Write short note on the following (any four): 4x5=20

    a) Hellmann-Feynmann theorem and its proof

    b) Density functional theory

    c) Zeeman Splitting

    d) Koopman's theorem

    e) Roothan equation

    f) Hartee-Fock SCF method

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