2018

CHEMISTRY

CHM 301

QUANTUM CHEMISTRY

Full Marks: 80

Time: 3 hours.

The figures in the margin indicate full marks for the questions

1 Write down the molecular wave function for H_2 in the LCAO-MO framework. How Heitler & London modify it? 1+1

2 Write down the steps to construct MOs of H_2O molecule. 3

3 Find the energy gape expression for the highest wavelength $\pi \rightarrow \pi^*$ transition for a linear conjugate system of $n + 1$ carbon atoms. 7

4 Discuss the LCAO-Mo treatment of H_2^+. 9

5 Write down the Hamiltonian for Helium atom& identify the perturbed term present in it. 2

6 Show that the first order correction to the wave function & energy can be determined from the Eigen function and Eigen value of the unperturbed system. 4+4

7 Using variation method, construct the Secular determinant for a system of function 5

$$\psi = a_1\varphi_1 + a_2\varphi_2$$

8 What are linear and non-linear variation functions? Find an expression for $\bar{E}$ for harmonic oscillator. 5

[Given $\psi = e^{-\beta x^2}$; $\int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$; $\int_{-\infty}^{+\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$; $\beta \rightarrow$ variable parameter]

9 From the variation treatment, find out the ground state energy of He atom. 7

10 State and explain Born-Oppenheimer Approximation. 3

11 Derive Hellmann-Feynmann theorem. 5

12 Explain Density functional theory based on Hohenberg-Kohn Theorems. Write the drawbacks of DFT. 6+2

13 Derive the wave function for n-electron system using SCF approximation. Discuss its application to He-atom. Also obtain the orbital energy and total energy term. 5+2+3

14 Write a short on 3+3

a) Roothaan's equation

b) Pariser-Parr-Pople Approximation

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