Total No. of printed pages = 3

63/2 (SEM-3) CHM 301

2022

(Held in 2023)

CHEMISTRY

(Theory Paper)

Paper Code : CHM-301

(Quantum Chemistry)

Full Marks – 80

Pass Marks – 32

Time – Three hours

The figures in the margin indicate full marks for the questions.

1. Answer any *three* of the following questions : 5×3=15

   (a) Deduce the Perturbation theory.

   (b) Apply Perturbation theory to the ground and first excited states of the Helium atom.

   (c) Describe briefly the Self-consistent field method.

   (d) Write briefly about the Hartee-Fock SCF method.

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(e) Write short notes on any *one* of the following :

(i) Koopman's theorem

(ii) Roothan equation.

2. Answer any *four* of the following questions : 10×4=40

(a) Explain the LCAO-MO treatment of H_2^+ ion and construct the LCAO-MO energy profile diagram of H_2^+ ion. 7+3=10

(b) Discuss the VB treatment of hydrogen molecule and construct the LCAO-MO energy profile diagram of hydrogen molecule. 7+3=10

(c) Explain the Huckel molecular orbital method for conjugated organic molecules. Write down the Secular determinant for benzene molecule. 5+5=10

(d) Write down the guidelines that are followed in the construction of hybrid orbitals. Explain for sp^3 hybridization. 4+6=10

(e) Write down the comparison between MO and VB treatment. Write down the guidelines for LCAO-MO treatment of triatomic molecules. 6+4=10

(f) Discuss LCAO-MO treatment of BeH_2. Write down the general expression of Huckel MO energy levels for cyclic polyenes. 7+3=10

3. Answer any *three* of the following questions : 5×3=15

(a) What is Zeeman splitting ? Explain the differences between normal and anomalous Zeeman effects. 2+3=5

(b) What are Racah and Condon-Shortly electron repulsion parameters ? Write down their applications. 2+3=5

(c) What are the possible term symbols of d^2 configuration ? Discuss the splitting of free ion terms of d^2 configuration due to J-S coupling. 2+3=5

(d) Explain Pauli's antisymmetric and exclusion principle. 5

(e) Write the brief short note on Spin orbit coupling. 5

4. Answer any *two* of the following questions : 5×2=10

(a) What is Hellmann-Feynmann theorem ?

(b) Write a short note on Density function theory.

(c) Discuss briefly about molecular electronic viral theorem.