

**M.Sc. DEGREE (C.S.S.) EXAMINATION, AUGUST 2015****Second Semester**

Faculty of Science

Branch : Chemistry

**AN2C07/AP2C07/CH2C07/PH2C07/POH2C07—CHEMICAL BONDING AND  
COMPUTATIONAL CHEMISTRY**

(Common to all branches of Chemistry)

(2012 Admission onwards)

Time : Three Hours

Maximum Weight : 30

**Section A***Answer any ten questions.**Each question carries a weight of 1.*

1. What is meant by free valance ?
2. In what respects the quantum mechanical harmonic oscillator differs from classical oscillator ?
3. Plot the radial portions of the 4s, 4p, 4d and 4f hydrogen like wave functions.
4. Explain the quantum mechanical treatment for Pauli's exclusion principle.
5. Calculate the average potential and kinetic energies of a harmonic oscillator in the ground state. Compare the results obtained with the classical results.
6. What are Slater determinants ?
7. Calculate the  $\pi$ -bond order for the excited state of butadiene.
8. Write down the Hamiltonian operator for electrons in hydrogen molecule and explain the terms involved.
9. Write down the Hückel determinants for benzene and butadiene.
10. What are the transformation properties of atomic orbitals ?
11. What is meant by Configuration Interaction ?
12. What are the basic principles of Møller Plesset Perturbation Theory ?
13. What is meant by Koopman's theorem ? What are its applications ?

(10 × 1 = 10)

**Turn over**

**Section B**

*Answer any five questions.*

*Each question carries a weight of 2.*

14. Discuss the qualitative idea of Hellmann-Feynman Theorem.
15. Explain the quantum mechanical treatment of  $sp$  and  $sp^2$  hybridizations.
16. Deduce the Hückel molecular orbitals for ethylene.
17. Give the systematic procedure for the determination of point groups.
18. Draw the MO diagrams of  $H_2O$  and  $NH_3$ .
19. Explain the Density Functional Theorem.
20. Discuss the general format of GAMESS.
21. Discuss the Hartee-Fock method.

(5 × 2 = 10)

**Section C**

*Answer any two questions.*

*Each question carries a weight of 5.*

22. What are Hermite polynomials ? How are they used in solving the Schrödinger equation for a harmonic oscillator ?
23. Construct the ground state wave function for  $H_2$  molecule according to VB method. Compare it with MO wave function.
24. Deduce the hybrid orbitals of  $BF_3$  and  $PCl_5$  molecules using group theoretical treatment.
25. What are the applications of Computation chemistry ?

(2 × 5 = 10)