

G 17003240



17003240

Reg. No.....

Name.....

**M.Sc. DEGREE (C.S.S.) EXAMINATION, JULY 2017**

**Second Semester**

Faculty of Science

Branch : Chemistry

AN2C07/AP2C07/CH2C07/PH2C07/POH2C07- CHEMICAL BONDING AND  
COMPUTATIONAL CHEMISTRY

(2012 Admission onwards)

[Common to all branches of Chemistry]

Time : Three Hours

Maximum Weight : 30

**Section A**

*Answer any ten questions.  
Each question carries weight 1.*

1. State and explain 'Gaussian orbitals'.
2. Draw the MO energy level diagram of  $O_2$  molecule.
3. What is Born-Oppenheimer approximation ?
4. Show that the ground state term symbol of hydrogen is  $^1\Sigma_g^+$ .
5. Apply SALC, to Ammonia molecule.
6. Of the species  $O_2$ ,  $O_2^+$ ,  $O_2^-$ ,  $O_2^{2-}$  which would have the maximum bond strength ?
7. Compare the bond energy, bond length and magnetic behavior of CN and  $CN^-$  species with the help of molecular orbital theory.
8. Write the Z-matrix of Ammonia.
9. What is ladder operator ? What is its use ?
10. State and explain the 'Noncrossing rule' in quantum mechanics.
11. Explain the notation MP2/6-31G (d, p)//HF/6-31G.
12. Explain Koopmans theorem.
13. What is MMFF ? What are its common features ?

(10 × 1 = 10)

Turn over





G 17003240

### Section B

*Answer any five questions.  
Each question carries weight 2.*

14. Write down the normalized valence bond wave function and molecular orbital wave function for  $H_2$  molecule and comment on the expressions obtained.
15. Apply Hückel Molecular Orbital (HMO) theory to 1, 3-butadiene.
16. Compare the molecular orbital theory (MOT) and valence bond theory (VBT). Give the merits and demerits of the two theories in explaining the properties of molecules. Compare Slater type orbitals and Gaussian orbitals. Give sketches of the two.
17. Write the basic concepts of Hartree-Fock Self Consistent Field (HFSCF) method.
18. Calculate the Symmetry adapted linear combination (SALC) to the stretching vibrations of  $D_{3h}$  molecule.
19. Write an input file for geometry optimization of Ammonia at HF/6-31G(d,p) level of theory followed by frequency calculation in GAMESS.
20. List the principles of Hohenberg-Kohn theorems? Explain the use of these theorems in Density Functional Theory (DFT) methods.
21. What are 'Generalized gradient approximation and local density approximations'?

(5 × 2 = 10)

### Section C

*Answer any two questions.  
Each question carries weight 5.*

22. Give the molecular orbital (MO) treatment for the following molecules.  
(a)  $N_2$                       (b)  $NO$                       (c)  $HF$ .
23. State and prove variation theorem and apply it to a particle in a one dimensional box using a suitable trial function.
24. Give the general format of GAMESS and explain : (a) Single point energy calculation ; and (b) Frequency calculation using suitable examples.
25. Using group theory explain the bonding in the following molecules :  
(a)  $PCl_5$                       (2)  $CH_4$ .

(2 × 5 = 10)

