

G 5858

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Reg. No.....

Name.....

M.Sc. DEGREE (C.S.S.) EXAMINATION, AUGUST 2013

Second Semester

Faculty of Science

Branch : Chemistry

AN 2C 07/AP 2C 07/CH 2C 07/PH 2C 07/PO 2C 07—CHEMICAL BONDING AND
COMPUTATIONAL CHEMISTRY

(2012 Admissions)

[Common to all branches of Chemistry]

Time : Three Hours

Maximum Weight : 30

Section A

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

1. What is basis functions ?
2. State variation theorem.
3. Explain any one qualitative idea obtained from Hellmann Feynman theorem.
4. State Born-Oppenheimer approximation.
5. In terms of the molecular orbital theory, explain the non-existence of He_2 .
6. Calculate the energy levels for benzene molecule using HMO theory.
7. Distinguish between SALC and SAGO.
8. Draw MO diagram for NH_3 .
9. Explain AMBER.
10. What is Kohn-Shann orbitals ?
11. What is Abinitio method ?
12. What are the guidelines for writing Z-matrices ?
13. Write down the Z-matrices of acetylene.

(10 × 1 = 10)

Section B

*Answer five questions.
Each question carries a weight of 2.*

14. Write note on HFSCF theory.
15. Explain Roothmans concept of basis function.
16. Discuss valence bond theory of H_2 molecule.
17. Give the quantum mechanical treatment of sp^3 hybridisation.

Turn over

18. How will you construct hybrid orbitals for CH_4 molecule?
19. Discuss different molecules mechanics methods.
20. Write a note on basis set.
21. Explain the notation (MPZ / 6-31 G (d, P // HF / 6-31 G).

(5 × 2 = 10)

Section C

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

22. Compare and contrast MO theory and VB theory with suitable example.
23. Apply perturbation method to He.
24. Compare the basic principles of the different computational methods in chemistry.
25. How is Gaussian input file prepared? Illustrate with reference to water molecule.

(2 × 5 = 10)