15·4

TM242437N

Reg. No :.....

Name :.....

MASTER'S DEGREE (C.S.S) EXAMINATION, MARCH 2024

2023 ADMISSIONS REGULAR

SEMESTER II - CORE COURSE CHEMISTRY

CH2C07TM20 - Chemical Bonding and Computational Chemistry

Time : 3 Hours **Maximum Weight : 30**

Part A

I. Answer any Eight questions. Each question carries 1 weight **(8x1=8)**

1. Discuss about distortions in octahedral molecule.
2. Write a note on transition moment integral.
3. Discuss orbital selection rule.
4. Account on the HFSCF method.
5. State and explain Shell model.
6. Sketch and explain the MO diagram of NO.
7. Discuss Schrodinger equation for molecules.
8. Schematically explain Saddle point, local minima and global minima.
9. Explain HF limit.
10. Describe briefly the semiempirical method used in computational chemistry.

Part B

II. Answer any Six questions. Each question carries 2 weight **(6x2=12)**

11. Explain in detail electronic transitions in C_{4h}
12. Discuss in detail electronic transitions in C_{4v}.
13. Give an account on Perturbation method.
14. Account on the first order correction to energy and wave function in time-independent perturbation method.
15. Discuss the MO treatment of H_2 molecule.
16. With the aid of suitable examples discuss the MO treatment of homonuclear diatomic molecules.
17. Discuss the advantages and disadvantages of ab initio method.
18. Write an input file for geometry optimization of water at HF/6-31g(dp) level of theory in GAMESS.

Part C

III. Answer any Two questions. Each question carries 5 weight **(2x5=10)**

19. Describe in detail electronic transitions in formaldehyde using group theory.
20. Discuss (i) Hellmann-Feynman theorem with its applications. (ii) Gaussian type orbitals.
21. Discuss Valence Bond theory as applicable to H_2 molecule.
22. Discuss the Density Functional Theory.