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Reg. No.....

Name.....

M.Sc. DEGREE (C.S.S.) EXAMINATION, JUNE 2018

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 weight-*1.

1. Draw the MO energy level diagram of N_2 molecule.
2. What is bond order ? How it is calculated ?
3. What is 'correlation diagram' as used in quantum mechanics.
4. Apply SALC to Water molecule.
5. What are 'Slater determinants' ?
6. Derive the spectroscopic term symbols for O_2.
7. Write the Z- matrix of Butane.
8. What is ladder operator ? What is its use ?
9. State and explain the 'Noncrossing rule' in quantum mechanics.
10. Explain the notation MP2/6-31G (d,p)//HF/6-31G.
11. Explain Hellmann-Feynman theorem.
12. What is CHARMM ? Explain its use in molecular mechanics.
13. Explain Kohn-Sham orbitals.

(10 × 1 = 10)

Turn over

Section B

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

14. What are the important assumptions used in the HFSCF method for the determination of the wave function and energy of a quantum many body systems in a stationery state.

15. What are the important problems faced in quantum mechanical calculations for many particles compared to a single particle ? How it is overcame ?

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.

17. Give the basic principles of Moller Plesset perturbation theory.

18. State and prove variation theorem and apply it to a particle in a one dimensional box using a suitable trial function.

19. Calculate the Symmetry adopted linear combination (SALC) to the stretching vibrations of C_{2h} molecule.

20. Write an input file for geometry optimization of Water at HF/6-31G (d,p) level of theory followed by frequency calculation in GAMESS

21. What are 'Generalized gradient approximation and local density approximations' ? Explain the basic principles.

(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.

    (1) Be_2 (2) NO.

    (3) LiH.

23. Compare the following calculations in quantum mechanics.

    (1) Density Functional Theory (DFT) methods.

    (2) ab initio methods.

    (3) Molecular mechanics method.

24. Give the general format of GAMESS and explain Basis set selection, method selection, charge, multiplicity, single point energy calculation and Frequency calculation.

25. Using group theory explain the bonding in the following molecules :

    (1) BF_3. (2) CH_4.

(2 × 5 = 10)