C 63027 **(Pages : 2)** **Name.....**

Reg. No.....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, JUNE 2019

(CUCSS)

Chemistry

CH 2C 05—APPLICATIONS OF QUANTUM MECHANICS AND GROUP THEORY

(2015 Admissions)

Time : Three Hours Maximum : 36 Weightage

Part A

Answer **all** *questions.*
Each question carries 1 weightage.

1. What is the many body problem faced in quantum mechanics ?
2. What is the spin orbital of an atom of electronic configuration $1s^2$?
3. Starting from the Slater determinant of Li atom, show that the maximum occupancy of an orbital is 2.
4. Define Coulomb and Exchange integrals.
5. How many independent electronic wave functions correspond to the diatomic molecular term n^3 ? Give the levels belonging to this term.
6. Write down the possible spin and orbital functions for the electronic configuration, $1s^1\,2s^1$ and construct its spin orbital.
7. How wil you calculate the n-bond order using Huckel theory.
8. Using Frost diagrams, predict the aromatidantiaromatic/non-aromatic nature of (i) cyclopropenyl cation ; (ii) Cyclopentadienyl cation ; (iii) Cyclobutadienyl diaction ; (iv) Cyclooctatetraenyl dianion.
9. What are vanishing and non-vanishing integrals ?
10. Write the Laporte rule.
11. What is SALC ? How will you construct this ?
12. What is transition moment integral ? What is its importance in spectroscopy ?

(12 x 1 = 12 weightage)

Part B

Answer any **eight** *questions.*
Each question carries 2 *weightage.*

13. Write down the Schrodinger equation of Helium atom. State the perturbation term from the corresponding Hamiltonian operator and calculate the first order correction to energy.

Turn over

14. Differentiate Hartree's and Hartree-Fock's proposal of trial wave function for a molecule. Enunciate the limitations of Hartree Fock method.

15. What are Gaussian Type orbitals ? How do they differ from hydrogenic orbitals ?

16. Derive the term symbols for 0_2 molecule and arrange them in the order of their energies.

17. Compare and contrast MOT and VBT treatment of 11_2 molecule.

18. Illustrate correlation diagrams with an example.

19. Explain the approximation incorporated in Hiickel theory. Write down the Htickel determinant of benzene and hexatriene. How do they differ ?

20. Calculate the delocalization energy of benzene using HMO method.

21. HCHO belongs to C_{2v} point group. Find the allowed electronic transitions of the molecule.

22. Use the 0_{2v} character table and transformp_x , p_y andp_z orbitals of oxygen in water to corresponding irreducible representations :

C2v	E	C_{2z}	$_v(xy)$	$a_v(yz)$
A_1	1	1	1	1
A_2	1	1	–1	–1
B_1	1	–1	1	–1
B_2	1	–1	–1	1

23. Write down the normalized expressions of *spa* hybrid orbitals of C in CH_4 and show that they are mutually orthogonal.

24. Construct the molecular orbital diagrams of CO, NO and 0_2. Compare the nature of bonding based on their bond orders.

(8 x 2 = 16 weightage)

Part C

Answer any two *questions.*
Each question carries 4 *weightage.*

25. State and prove variation theorem. Calculate the variation energy for the following trial function for particle in a box of length, a ; (1)(x) = *x(a-x).*

26. Outline the solution of the Schrodinger equation for H_2 molecule within the valence bond theory approximation.

27. Explain in detail the Hartree Fock self consistent field method for atoms.

28. Find out the total molecular vibrations of H_2O molecule using C_{2v} character table. Identify the IR and Raman activity of these vibrations.

(2 x 4 = 8 weightage)