18P213 (Pages: 2) Name………….……….

Reg. No……….………..

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2019
(Regular/Supplementary/Improvement)

(CUCSS – PG)

CC15P CH2 C05 - APPLICATIONS OF QUANTUM MECHANICS AND GROUP THEORY
(Chemistry)

(2015 Admission onwards)

Time: Three Hours   Maximum:36 Weightage

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

1. What do you mean by first order perturbation method? Explain.
2. Write down the Hamiltonian operator for the Li atom, in a.u.
3. What is Fock operator?
4. Write down the slater determinantal wave function for He atom in the ground state.
5. State and Explain non-crossing rule.
6. Differentiate between SALC and SAGO.
7. Write the spectroscopic term symbol for N_2.
8. Arrange O_2, O_2^+ and O_2^- in the increasing order of stability. Justify your answer.
9. You are given the integral $\int_{-a}^{+a} x^3 dx$. Check whether it is a vanishing integral or not.
10. Explain transition moment integral. How does it help in predicting spectroscopic transition?
11. What is Pauli's antisymmetric principle?
12. Use the projection operator method to find the symmetry species of 1S – orbitals of H-atoms of water molecule. Use the character table in question no.21.

(12 x 1 = 12 Weightage)

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

13. Find out the ground state energy and wave function of He atom using variation theorem (Hint J =5/8Z, $\int_0^\infty r exp(-2Zr) dr = 1/2Z^2$)
14. Discuss the Frost -Hückel circle mnemonic device for cyclic polyenes.
15. Briefly discuss the Roothan's concept of basis functions.
16. Write a brief note of quantum mechanical treatment of sp^2 hybridization.
17. Taking bonding in NO, draw correlation diagram. Discuss.
18. Write the four possible spin and orbital combinations of ground state of He atom. Which one will be true representation of the ground state?

19. Compare the VB and MO treatment of molecules.

20. Explain HMO treatment of butadiene, to find the π bond energy.

21. HCHO belongs to C_{2v} point group. Find the symmetry species of MO's. (You may neglect S-orbitals)

C_{2v}	E	C2	σv	$\sigma v'$
A1	1	1	1	1
A2	1	1	-1	-1
B1	1	-1	1	-1
B2	1	-1	-1	1

22. Explain the term Inverse transformation.

23. Rationalize the rule of mutual exclution principle using group theory.

24. Using C_{3V} character table find out E⊗E and reduce it.

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2,\ z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y),\ (R_x,\ R_y)$	$(x^2 - y^2,\ xy),\ (xz,\ yz)$

(8 x 2 = 16 Weightage)

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

25. Find the IR and Raman active vibrations of CH_4 molecule. Use the T_d character table given below.

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	linear functions, rotations	quadratic functions
A_1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$
A_2	+1	+1	+1	-1	-1	-	-
E	+2	-1	+2	0	0	-	$(2z^2-x^2-y^2,\ x^2-y^2)$
T_1	+3	0	-1	+1	-1	$(R_x,\ R_y,\ R_z)$	-
T_2	+3	0	-1	-1	+1	$(x,\ y,\ z)$	$(xy,\ xz,\ yz)$

26. Illustrate variation theorem using the trial wave function as $e^{-\alpha r^2}$ for hydrogen atom.

27. Discuss briefly the self consistent filed method of solving many electron atoms.

28. Taking H_2 as an example compare and contrast VB and MO theory.

(2 x 4 = 8 Weightage)

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