16P210

Name.................

Reg.No.................

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, MAY 2017
(Regular/Supplementary/Improvement)

(CUCSS – PG)

(Chemistry)

CC15P CH2 C05 - APPLICATIONS OF QUANTUM MECHANICS AND GROUP THEORY

(2015 Admission Onwards)

Time: Three Hours

Maximum:36 Weightage

Section A *Answer all questions (1 weightage)*

1. What is variation Theorem
2. Write down the slater determinant for Li atom.
3. What is Born-Oppenheimer approximation?
4. What is fock operator.
5. What is Roothan's concept of basis function.
6. Differentiate between STO and GTO.
7. Write the spectroscopic term symbol for C_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 $\int_{-a}^{+a} x^2 dx$. Check whether it is a vanishing integral or not.
10. Explain transition moment integral. How does it help in predicting spectroscopic transition?
11. State non crossing rule as applied to correlation diagrams.
12. Write the projection operator P_{A1} for C_{2V}.

(12x1=12 Weightage)

Section B *(Answer any eight questions) (2 weightage)*

13. Using the trial wave function for the ground state of particle in a 1-D box as $x^2(x-a)^2$ find out the energy using variation theorem. Does it represent the true ground state energy?
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^3 hybridization
17. Taking bonding in CO 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 ethylene, to find the π bond energy.

21. H_2O belongs to C_{2v} point group. Find the symmetry species of MO's and arrange them.

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

22. Using group theory rationalize rule of mutual exclusion principle.

23. How do you explain Laporte selection rule using group theory.

24. Using $2P_x$ orbital on Cis butadiene find out the reducible representation and reduce it to irreducible representation. Use the C_{2v} character table in question 21.

(8x2=16 Weightage)

Section C *(Answer any two questions) (Weightage 4)*

25. Find the hybridization and molecular orbital diagram 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. Find out the ground state energy and wave function of He atom using variation theorem (Hint J $=5/8Z$ $\int_0^\infty rexp(-2Zr)dr =1/2Z^2$).

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

28. Discuss briefly the LCAO method of bonding applied to hydrogen molecule ion.

(2x4=8 Weightage)

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