17P215 (Pages: 2) Name…….

Reg. No……..

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, MAY 2018

(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. State variation theorem.
2. Write down the slater determinant for Li atom.
3. Write down the Schrodinger equation for H_2 molecule.
4. What is Fock operator?
5. What is Roothan's concept of basis function?
6. Write down the spectroscopic term symbol for N_2 molecule.
7. Discuss charge density and free valence for conjugated systems
8. What is Frost –Huckel Circle Mnemonic device for cyclic polyenes?
9. ∫ x3 dx (limit -a to+a) Find out whether it is a vanishing integral or not? Justify your answer.
10. State non crossing rule as applied to correlation diagrams
11. Construct projection operator of B_1 representation for hydrogen is orbitals of H_2O molecule belonging to C_{2v} point group.
12. What is transition moment integral?

(12 x 1 = 12 Weightage)

Section B

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

13. Illustrate how perturbation method is applied to particle in a ID box with slanted bottom.
14. How is variation method applied to calculate the energy of the ground state of He atom?
15. Write a brief account of quantum mechanical treatment of sp hybridization.
16. Distinguish STO and GTO.
17. Assign symmetry species for the molecular orbitals in H_2O. Find allowed electronic transitions. Use C_{2v} character table given below.
18. Using group theory rationalize the complimentary character of IR and Raman spectra.

19. How do you explain Laporte selection rule using group theory?
20. Draw the MO diagram for CO and NO and compare their bond order.
21. State and explain Born –Oppenheimer approximation. Discuss its significance.
22. Find the hybridized orbitals of C in CH_4 molecule. Character table of Td is given.

Td	E	8C3	3C2	6S4	6σd		
A1	1	1	1	1	1		$x^2+y^2+z^2$
A2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z2-x^2-y^{2,x2-y2)}$
T1	3	0	-1	1	-1	R_x,R_y R_z	
T2	3	0	-1	-1	1	x,y.z	xz,xy,yz

23. Explain how projection operator can be used for constructing SALCs for the π MOs in cyclopropenyl cation $(C_3H_3)^+$ cation.

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

24. Explain molecular orbital theory of benzene molecule using Huckel determinants.

(8 x 2 = 16 Weightage)

Section C

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

25. Set up the Huckel determinant of butadiene and obtain their energies and coefficient of the π molecular orbitals.
26. Discuss Hartree –Fock self consistent field method for atoms.
27. Explain how group theory helps in predicting IR and Raman active vibrations in H_2O molecule.

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

28. Compare VB and MO methods for explaining bonding in H_2 molecule

(2 x 4 = 8 Weightage)

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