19P211 (Pages: 2) Name…………………………

Reg. No....………………..

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2020

(CUCSS - PG)

CC19P CHE2 C05 - GROUP THEORY AND CHEMICAL BONDING

(Chemistry)

(2019 Admissions - Regular)

Time: Three Hours Maximum: 30 Weightage

Section A (Short Answer Type)

Answer any ***eight*** questions. Each question carries 1 weightage.

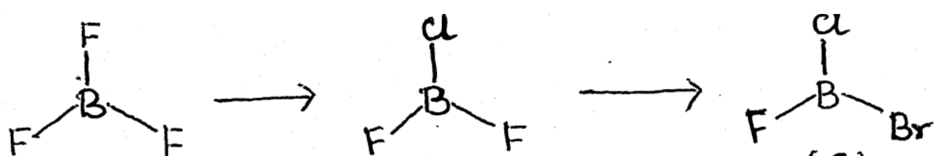
1. Write down the 3 × 3 matrix for S_2 and find out its equivalent symmetry operation.
2. What is rearrangement theorem?
3. Draw the structures of three distinct isomers of $C_2H_2Cl_2$ and determine their point group. Which of them is polar?
4. What are orthogonal matrices? What is its property?
5. What is Laporte selection rule in terms of group theory?
6. Differentiate between SALC and SAGO.
7. How will you calculate the π bond order using Huckel theory?
8. What is the term symbol for N_2 molecule?
9. Show that B_1 and B_2 IR's under C_{2v} point group is mutually orthogonal. (Use the character table in question number 18)
10. State and explain Born-Oppenheimer approximation.

(8 × 1 = 8 Weightage)

Section B (Short Essay Question)

Answer any ***four*** questions. Each question carries 3 weightage.

11. A point group has the following irreducible representations: A_1, A_2, B_1, B_2, E_1, E_2. What is the order of the group? How many classes are there in that group? Justify your answer.
12. Consider the following sequential changes from A to B and to C. 1) Indicate the point group of each of these structures 2) List out the symmetry elements that are lost or gained during this transformation from A to C.



(A) (B) (C)

13. Explain the four different properties of IR's derived from GOT.

14. Write a brief note of quantum mechanical treatment of sp^3 hybridization
15. Discuss the Frost -Hückel circle mnemonic device for cyclic polyenes.
16. Explain the rule of mutual exclusion principle using group theory.
17. HCHO belongs to C_{2v} point group. Find the allowed electronic transiotions in the C=O group of this 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

(4 × 3 = 12 Weightage)

Section C (Essay questions)

Answer any ***two*** questions. Each question carries 5 weightage.

18. Sate Great Orthogonality Theorem. Using this derive the C_{3V} character table.
19. Compare the VB and MO method of bonding applied to H_2. Which is found better? Justify your answer.
20. a) Explain the basics of Huckel approximations. How are these justified?
    b) Obtain the secular determinant for cyclobutadiene, find out the MO and calculate the delocalization energy based on Huckel approximation.
21. Consider a general vector v whose base is at the origin of the coordinate system and whose tip is at (x, y, z) in the point group C_2V.
    a) Derive the set of four 3×3 transformation matrices that constitute the reducible representation by which vector v transforms.
    b) From this find out the IR for the transformation of x, y, and z under this point group.
    c) Derive the complete character table for this point group.

(2 × 5 = 10 Weightage)

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