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Name.....

Reg. No.....

SECOND SEMESTER M.Sc. (CBCSS) REGULAR/SUPPLEMENTARY DEGREE
EXAMINATION, APRIL 2024

Chemistry

CHE 2C 05—GROUP THEORY AND CHEMICAL BONDING

(2019 Admission onwards)

Time : Three Hours

Maximum Weightage : 30

Section A

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

1. Assign Schoenflies symbol of point group for (a) Pyridine ; (b) Ethane (staggered conformation).
2. Generate 3×3 matrices for (a) C_4 ; (b) S_4 .
3. Distinguish between reducible and irreducible representations with examples.
4. State and explain rearrangement theorem.
5. Distinguish between Vanishing and Nonvanishing integrals with example.
6. Two vertical planes of water molecule belong to different classes of operations but the three vertical planes of ammonia belong to the same class. Why ?
7. State and explain Born-Oppenheimer approximation.
8. NO^+ is more stable than Na but NO^+ is less stable than CO. Why ?
9. Write spectroscopic term symbol for the ground. State of (a) B_2 ; (b) O_2^+ .
10. Explain the term 'free valence' with reference to conjugated systems.

(8 × 1 = 8 weightage)

Section B

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

11. List symmetry elements and operations associated with D_{2h} . Classify them into different classes of operations.
12. Develop Gamma chart for H_2O (C_{2v} point group).
13. State Great orthogonality theorem. What are the consequences of the theorem ? Discuss.

Turn over

14. Predict allowed electronic transitions of formaldehyde. Use C_{2v} character table

C_{2v}	E	C_{2z}	σ_{vxx}	σ'_{vyz}		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	Rz	xy
B_1	1	-1	1	-1	x, Ry	xz
B_2	1	-1	-1	1	y, Rx	yz

15. Use HMO method to find the P_1 (π) molecular orbitals and the corresponding allyl anion.
 16. Briefly discuss sp^2 hybridization to find the composition of hybridized orbitals
 17. Explain with example direct product representations.
 18. Reduce the following representation 'T' into its IR components. Use C_{2v} char (Question No.14)

C_{2v}	E	C_{2z}	σ_{vxx}	σ'_{vyz}
T	9	-1	1	3

(6 × 2 = 12)

Section C

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

19. Find IR and Raman active vibrations of CH_4 . Use T_d character table :

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
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	(Rx, Ry, Rz)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)

20. Compare V.B. and M.O. method of bonding as applied to H_2 . Which is found better? Justify your answer.
21. What are the assumptions in HMO method? Use the theory to find the molecular orbitals and the corresponding energies for benzene.
22. Discuss briefly :
- (a) Mutual exclusion principle from group theoretical point of view.
 - (b) Correlation diagram applied to bonding.
- (2 × 5 = 10 weightage)