

D 102125

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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  $3 \times 3$  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	$C_{2z}$	$\sigma_{vzx}$	$\sigma'_{vyz}$		
$A_1$	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  $P_1$  ( $\pi$ ) molecular orbitals and the corresponding energies of 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  $C_{2v}$  character table (Question No.14)

$C_{2v}$	E	$C_{2z}$	$\sigma_{vzx}$	$\sigma'_{vyz}$
T	9	-1	1	3

(6 × 2 = 12 weightage)

### Section C

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

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

Td	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)

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)