D 140643 **(Pages : 3)** **Name.....**

Reg. No.....

SECOND SEMESTER M.Sc. (CBCSS) REGULAR/SUPPLEMENTARY DEGREE EXAMINATION, APRIL 2026

Chemistry

CHE2C05—GROUP THEORY AND CHEMICAL BONDING

(2019 Admission onwards)

Time : Three Hours Maximum Weightage : 30

Part A

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

1. Assign Schoenflies symbol of point group for (a) Cyclohexane (boat form) ; (b) Ethane (eclipsed conformation).
2. Generate 3 × 3 matrices for (a) σ_{hxy} ; (b) inversion.
3. Show that $S_2^1 = i$ (inversion).
4. Distinguish between inverse operation and conjugate operation.
5. You rare given $\int_{-a}^{+a} x^2 dx$. Predict whether it is vanishing integral or not. Justify.
6. State and explain rearrangement theorem.
7. Write projection operator $\hat{P}_{A_1}$ for A_1 symmetry under c_{2v} point group.
8. State and explain Born-Oppenheimer approximation.
9. Write spectroscopic term symbols for (a) N_2 ; (b) O_2^-.
10. Explain the term 'free valence' with reference to conjugated systems.

(8 × 1 = 8 weightage)

Part B

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

11. List symmetry elements and operations associated with D_{3d}. Classify them into different classes of operations.

Turn over

12. Taking the positional co-ordinates of all atoms of cis butadiene (c_{2v}) generate a reducible representation (characters only).
13. State great orthogonality theorem. What are the consequences of the theorem ? Discuss.
14. Predict IR and Raman active vibrations of NH_3. Use C_{3v} character table :

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	Rz	
E	2	−1	0	(x, y) (Rx, Ry)	$(x^2 - y^2, xy)(xz, yz)$

15. Reduce the following representation T into its IR components :

C_{2v}	E	C_{2z}	σ_{vxz}	$\sigma'_v yz$		
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
	9	−1	1	3		

16. With the help of correlation diagram explain noncrossing rule.
17. Explain with example 'Direct product representation'.
18. Find the hybridized orbitals of C in CH_4 from quantum mechanical approach.

(6 × 2 = 12 weightage)

Part C

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

19. Find hybridized orbitals of B in BF_3. Use D_{3h} character table.

D_{3h}	E	C_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	Rz	
E^1	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	(Rx, Ry)	(xz, yz)

20. Briefly discuss VB theory of bonding as applied to H_2.

21. What are the assumptions in HMO method. Use the theory to find the π (pi) molecular orbitals and the corresponding energy values for allyl anion.

22. Discuss briefly :

    (a) Block diagonalization.

    (b) Material exclusion principle from group theoretical point of view.

(2 × 5 = 10 weightage)