25P210 (Pages: 3) Name: .....

Reg.No: .....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2026

(CBCSS - PG)

(Regular/Supplementary/Improvement)

CC19PCHE2C05 - GROUP THEORY AND CHEMICAL BONDING

(Chemistry)

(2019 Admission onwards)

Time : 3 Hours Maximum : 30 Weightage

Section A

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

1. What is meant by the term inverse of a group element? What is the inverse of the element C_3?
2. State and explain rearrangement theorem of group multiplication tables.
3. Give example of molecules with point groups: (i) C_1 (ii) C_s (iii) $D_{\infty h}$ (iv) D_{2d}.
4. What is meant by direct product of irreducible representations (IR)? Explain with example.
5. Write down the 3 × 3 matrix corresponding to symmetry operation C_3^2 in C_{3v} point group.
6. Show that all IR's under C_{2h} point group are mutually orthogonal.
7. Using the reduction formula reduce, reducible following represenations, Γ_a *and* Γ_b of C_{3v} point group into irreducible representation of the point group.

C_{3v}	E	$2C_3$	3σ
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
Γ_a	5	2	-1
Γ_b	7	1	-1

8. How many vibrational modes can occur in NH_3 molecule? Sketch all these modes.
9. Define Laporte selection rule. Explain.
10. Give the Hamiltonian for H_2 molecule. Explain the terms.
11. Differenciate between SALC and SAGO. Explain.
12. Give the Huckel matrix for benzene molecule.

(8 × 1 = 8 Weightage)

Section B

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

13. What are vanishing and non-vanishing integrals? How does it help in predicting spectroscopic transitions?

14. Explain how projection operator can be used for constructing SALCs for the π-MOs in cyclopropenyl cation $(C_3H_3)^+$ cation. (D_{3h}Table is given).

15. Depict all symmetry elements in PCl_5.

16. Describe the MO approach in the formation of LiH.

17. How does VB theory and MO theory make use of LCAO method? Explain.

18. Obtain the expressions for the energies of π-MOs ofbutadiene based on HMO theory.

19. Give the pictorial representation of π-MOs of benzene based on HMO theory.

(4 × 3 = 12 Weightage)

Section C

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

20. State Great Orthogonality Theorem. What are its consequences? Using this derive the C_{4v} character table.

21. By fixing three cartesian coordinates on each atom, find out the symmetries of vibrational modes of trans-dichloroethylene. Find IR and Raman activities of fundamental vibrational modes and prove rule of mutual exclusion principle. (C_{2h}Table is given).

22. Compare VB and MO treatments for explaining the bonding in H_2 molecule.

23. Explain MO diagram of water molecule using Group theory. (C_{2v}Table is given).

(2 × 5 = 10 Weightage)

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Refer Character table for required questions:

Character table for C_{2v} point group

	E	C_2 (z)	σ_v(xz)	σ_v(yz)	linear, rotations	quadratic
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

Character table for C2h point group

C_{2h}	E	C_2 (z)	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x or R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x or y	

Character table for D_{3h} point group

	E	$2C_3$	$3C'_2$	σ_h	$2S_3$	$3\sigma_v$	linear, rotations	quadratic
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)