

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2025
(Regular/Improvement/Supplementary)

CHEMISTRY
FCHE2C05: GROUP THEORY AND CHEMICAL BONDING

Time: 3 Hours

Maximum Weightage: 30

Section A: Short answer questions. Answer any *eight* questions. Each carries 1 weightage.

1. Generate matrices for C_6 and S_6 .
2. List out all the symmetry elements and operations associated with a T_d molecule.
3. Give the point group of: i) staggered ethane; ii) allene.
4. What are vanishing and non-vanishing integrals.
5. Explain the importance of reduction formula in group theory.
6. State the rules for assigning Mulliken's symbol for irreducible representation.
7. What is meant by symmetry adapted linear combinations of orbitals?
8. State Laporte selection rule for centrosymmetric molecules.
9. Write the trial wave function to understand bonding in H_2 in the VB method.
10. Write the molecular orbital configuration for NO. Find the bond order.
11. What is the term symbol for the first excited state of H_2 molecule?
12. Explain the term free valance on a carbon atom in a conjugated system.

(8 × 1 = 8 weightage)

Section B: Short essay questions. Answer any *four* questions. Each carries 3 weightage.

13. Set up the group multiplication table for C_{3v} point group.
14. Discuss the rules to be obeyed for a set of elements to form a mathematical group.
15. State the great orthogonality theorem. Explain how it is helpful in constructing the character table with an example?
16. Using group theory rationalize rule of mutual exclusion principle.
17. Find the group orbitals involved in bonding with O atom orbitals of H_2O molecule.
18. Show that the character of the direct product matrix of two square matrices is equal to the product of characters of the individual matrices.
19. Briefly explain the quantum mechanical treatment of sp^2 hybridization.

(4 × 3 = 12 weightage)

(P.T.O.)

Section C: Essay questions. Answer any two questions. Each carries 5 weightage.

20. HCHO belongs to C_{2v} point group. Using group theory, find out the lowest energy electronic transition.
21. Set up the Huckel determinant of allylic anion and obtain their energies and wave functions of the π molecular orbitals.
22. Explain how group theory enables one to construct the hybrid orbitals of molecules taking BF_3 as an example.
23. Discuss the MO treatment of H_2^+ ion.

(2 × 5 = 10 weightage)

Character table of C_{2v} and D_{3h} point groups

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

D_{3h}	E	$2 C_3$	$3 C_2'$	σ_h	$2 S_3$	$3 \sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1	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)