D2ACH2101 **(2 Pages)** **Name.....**
Reg.No.....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2022
(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. Give the secondary rotational axes present in the molecule with the principal axes C_3.
2. Draw the structure of a molecule that contains only i and σ.
3. Give the point group of benzene, PCl_3, BF_3 and naphthalene.
4. How do you distinguish C_{nv} and C_{nh} point groups?
5. Differentiate reducible and irreducible representations.
6. What are the conditions for block-factorization of matrices?
7. What is the significance of orthogonality rule?
8. Define transition moment integral.
9. What are group orbitals?
10. Write the spectroscopic term symbol for O_2^+ molecule.
11. How can you calculate free valance from HMO parameters?
12. Write the Huckel determinant for benzene.

(8 × 1 = 8 weightage)

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

13. Show that there are four different classes in C_{2v} point group.
14. Construct the character table for C_{2v} point group.
15. Reduce the following into a combination of IRs.

C_{2v}	E	C_2	σ_{xz}	σ_{yz}
RR	12	-2	-2	12

16. Compare quantum mechanical treatment of VB and MO theories.

(P.T.O.)

17. Explain MO treatment of CO and NO.
18. Discuss quantum mechanical treatment of sp hybridization.
19. Explain the allowed an forbidden electronic transition in formaldehyde using group theory.

(4 × 3 = 12 weightage)

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

20. Construct hybrid orbitals of BF_3 molecule through inverse transformation procedure.
21. Construct the SALCs for the MOs in cyclopropenyl ($C_3H_3^+$) cation.
22. Determine the IR active and Raman active modes of ammonia molecule.
23. Discuss HMO theory with butadiene as an example.

(2 × 5 = 10 weightage)