D2ACH2001 **(2 Pages)** **Name.....**
Reg.No.....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2021
CHEMISTRY
FCHE2C05: GROUP THEORY AND CHEMICAL BONDING

Time: 3 Hours **Maximum Weightage: 30**

Section A: Short answer questions. *All* questions can be answered. Each carries *one* weightage (Ceiling 6 weightage).

1. Prove that all the cyclic groups are abelian where as the reverse is not true.
2. What is rearrangement theorem? Using this write the GMT for C_4.
3. Find out the point group of:
   a) Naphthalene, b) H_2O_2, c) Cyclohexane (chair), d) *o*-dichloro benzene.
4. What is similarity transformation? Prove that if element A is conjugate with element B, then B is also conjugate with A.
5. What is meant by block diagonalization of matrices?
6. What is rule of mutual exclusion principle?
7. Explain the concept 'group orbitals.'
8. By using the 3×3 matrix prove that C2 is its own inverse.
9. What is non-crossing rule?
10. Account for the triple bond in CO by MO method.
11. Write singlet and triplet state wave function of H_2 molecule in accordance with VBT.
12. Differentiate Finite and Infinite groups.

Section B: Short essay question. *All* questions can be answered. Each carries *four* weightage (Ceiling 12 weightage).

13. List out all the symmetry elements of T_d point group.
14. Write a brief note of quantum mechanical treatment of sp^2 hybridization.
15. Construct a character table for C_3 group.
16. Explain Laporte selection rule using group theory.
17. Explain the direct product and direct sum of square matrices.

(PTO)

18. Briefly discuss the Huckel Molecular Theory of benzene.
19. Using C_{3V} character table find out E⊗E and reduce it using symmetric direct product and ordinary direct product.

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	R_z	
E	2	-1	0	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

Section C: Essay questions. Answer *All* questions can be answered. Each carries *six* weightage (Ceiling 12 weightage).

20. Set up the secular equation for allyl system and solve Huckel Molecular orbital energies. Determine the coefficient of three Huckel molecular Orbitals.
21. State Great Orthogonality Theorem (GOT) and explain the terms. List its consequences.
22. Construct the SALCs for MOs in cyclopropenyl cation.
23. Find out the vibrational modes of NH_3 and predict which of these are IR and Raman active (use the character table in question No. 19).