SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2023
(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.   State and explain non-crossing rule.

2.   What is the resulting point group by combining inversion to C_{4v} point group?

3.   Write a short note on inverse transformation procedure.

4.   What is Frost-Huckel Circle Mnemonic device for cyclic polyenes?

5.   Write down the spectroscopic term symbol for O_2 molecule.

6.   State and explain Born-Oppenheimer approximation.

7.   What is an Abelian group? Give an example.

8.   Write MO electronic configuration of N_2 molecule and calculate its bond order.

9.   What sets of elements have to be added to convert C_{nh} point group into D_{nh}? Explain.

10. Write down 3 x 3 matrices corresponding to all symmetry operations in C_{2v} point group.

11. What is meant by transition moment integral?

12. Using the reduction formula reduce, reducible following representations, 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 × 1 = 8 weightage)

(P.T.O.)

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

13.   What meaning is implied in the Mulliken symbols A_g, B_u and B_g in C_2h point group.

14.   HCHO belongs C_{2v} point group. Find the symmetry species of MO's (you may neglect S-orbitals).

	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

15.   A Point group has the following irreducible representations: A_1, A_2, B_1, B_2, E_1, E_2. What is the order of the group? How many classes are there in that group? Justify your answer.

16.   Write a brief note on quantum mechanical treatment of sp^3 hybridization.

17.   Discuss the rules to be obeyed for a set of elements to form a mathematical group.

18.   How do you explain Laporte selection rule using group theory?

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

(4 × 3 = 12 weightage)

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

20.   Set up the Huckel determinant of butadiene and obtain their energies and coefficient of the π molecular orbitals.

21.   Using projection operator method construct MO for $C_3H_3^+$.

22.   Compare the VB and MO method of bonding applied to H_2 molecule. Which is found better? Justify your answer.

23.   State Great Orthogonality Theorem. Using this derive C_{2v} character table. Also include the IR corresponding to the vectors x, y, z and their products.

(2 × 5 = 10 weightage)