

20P211

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Name:

Reg. No:

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2021

(CUCSS - PG)

(Regular/Supplementary/Improvement)

CC19P CHE2 C05 - GROUP THEORY AND CHEMICAL BONDING

(Chemistry)

(2019 Admission onwards)

Time: Three Hours

Maximum: 30 Weightage

Section A

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

1. What are cyclic groups? Give an example.
2. What is rearrangement theorem in writing the group multiplication table?
3. Find out the point group of a) H_2O_2 (trans) b) diborane c) Ferrocene (eclipsed), d) cyclohexane (boat form)
4. What is similarity transformation? Prove that C_3 and C_3^2 are conjugate.
5. What is the resulting point group by combining inversion to C_{4v} point group?
6. Infrared and Raman activity of normal modes of trans N_2F_2 are mutually exclusive. Explain.
7. What is inverse transformation procedure?
8. By using the 3×3 matrix prove that C_3 is not its own inverse.
9. What is non-crossing rule?
10. Account for the triple bond in CO by MO method.

(8 × 1 = 8 Weightage)

Section B

Answer any *six* questions. Each question has 2 weightage.

11. Consider a general vector v whose base is at the origin of the coordinate system and whose tip is at (x, y, z) in the point group C_{2h} . Derive the set of four 3×3 transformation matrices that constitute the reducible representation by which v transforms
12. Write a brief note of quantum mechanical treatment of sp^2 hybridization
13. Discuss the Frost -Hückel circle mnemonic device for cyclic polyenes.
14. Explain Laporte selection rule using group theory.
15. What are vanishing and non-vanishing integrals? How does it help in predicting spectroscopic transitions?

16. Find out the transformation matrix for different symmetry operations of the four P_y orbitals, of cis-butadiene which are perpendicular to the plane of the molecule.

17. Using C_{3v} character table find out $E \otimes E$ and reduce it.

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	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

18. Discuss the MO treatment of LiH.

(6 × 2 = 12 Weightage)

Section C

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

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

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

21. Briefly discuss the HMO theory of benzene.

22. 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. 17)

(2 × 5 = 10 Weightage)
