23P210

Name: ....

Reg.No: ....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2024

(CBCSS - PG)

(Regular/Supplementary/Improvement)

CC19P CHE2 C05 - GROUP THEORY AND CHEMICAL BONDING

(Chemistry)

(2019 Admission onwards)

Time : 3 Hours

Maximum : 30 Weightage

Section A

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

1. What are cyclic groups? Give an example.

2. Using corresponding matrices, find equivalent symmetry operation corresponding to $C_2 \times \sigma_h$.

3. A point group has X number of 1D and 2D irreducible representations. Order of the group is 10. What is the value of X?

4. Using the reduction formula reduce, reducible following represenations, 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

5. Define Laporte selection rule. Explain

6. Find the hybridisation involved in H_2O molecule using C_{2V} character table.

7. What is the essential feature of VB theory?

8. What is non-crossing rule?

9. Obtain the energies of π-MOs of allyl anion based on HMO theory.

10. Calculate the π-bond order and free valence on the carbons in allyl anion.

11. Give the Huckel matrix for benzene molecule.

12. Diffrenciate between SALC and SAGO. Explain

(8 × 1 = 8 Weightage)

Section B

Answer any *four* questions. Each question carries 3 weightage.

13. Taking tans-dichloroethylene molecule, derive group multiplication table for C_{2h}.

14. Depict all symmetry elements in PCl_5.

15. 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_{2v}. Derive the set of four 3×3 transforms transformation matrices that constitute the reducible representation by which v transforms

16. Find the symmetries of vibrational modes of water molecule. Depict the transformation of these vibrational modes under each symmetry operation and assign symmetries to each vibrational mode.

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

18. Water belongs to C_{2v} point group. Find the symmetry species of MO's.

19. Discuss the theoretical interpretation of sp hybridization.

(4 × 3 = 12 Weightage)

Section C

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

20. State Great Orthogonality Theorem. Using this derive the C_3 character table. Also find the IRs corresponding to the vectors x, y, z and their products.

21. By fixing three cartesian coordinates on each atom, find out the symmetries of vibrational modes of $POCl_3$ molecule and predict which of these are IR and Raman active. Use C_{3v} character table.

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

23. Compare VB and MO treatments for explaining the bonding in H_2 molecule.

(2 × 5 = 10 Weightage)

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