22P210 (Pages: 2) Name: .....

Reg.No: .....

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2023

(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. Write the four important rules of mathematical groups.
2. Define rearrangement theorem of group multiplication tables (GMTs) and complete the GMT for a group having order 3 (G3).
3. What is meant by the inverse of a matrix?
4. Write down the matrix representation of $C_2(z)$ operation performed on unhybridized orbitals of 1,3-butadiene.
5. Write reduction formula to reduce reducible representation. Explain each term.
6. Find the symmetries of rotational vectors R_x and R_z in C_{2h} point group.
7. Find the hybridisation involved in NH_3 molecule using C_{3V} character table.
8. What are the factors that determine the energy of a MO?
9. Give the MO diagram of CO.
10. Obtain the energies of π-MOs of ethene based on HMO theory.
11. What is variation theorem?
12. Give the trial functions for sp, sp^2 and sp^3 hybridizations.

(8 × 1 = 8 Weightage)

Section B

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

13. Determine the symmetry elements present in at least four of the following molecules and assign the point groups (a) NH_3 (b) CO_3^{2-} (c) SiF_4 (d) HCN (e) SiFClBrI (f) BF_4^-
14. What are the rules for assigning Mulliken symbols to irreducible representations? Assign Mulliken symbols to all irreducible representations of C_{2h} point group.

15. Find the symmetries of vibratinal modes of ammonia molecule. Depict the transformation of these vibrational modes under each symmetry operation and assign symmetries to each vibrational mode.

16. Obtain the energies of π-MOs of benzene based on HMO theory.

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

18. Explain Born – Oppenheimer approximation taking H_2 as an example.

19. How does VB theory and MO theory explain the electronic configuration of molecules? Explain.

(4 × 3 = 12 Weightage)

Section C

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

20. Sate Great Orthogonality Theorem. Using this derive the C_{2v} 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 vibrational modes of H_2O and predict which of these are IR and Raman active. Use C_{2v} character table.

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

23. Discuss the theoretical interpretation of sp^3 hybridization.

(2 × 5 = 10 Weightage)

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