### SECOND SEMESTER M.Sc. DEGREE EXAMINATION, APRIL 2022
(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. Which sets of elements have to be added to convert $C_{nh}$ point group into $D_{nh}$? Explain.

2. What are orthogonal matrices? What are its properties?

3. Write down the 3 × 3 matrices corresponding to all symmetry operations in $C_{2v}$ point group

4. Using the reduction formula reduce, reducible following represenations, $\Gamma_a$ *and* $\Gamma_b$ of $C_{3v}$ point group nto irreducible representation of the point group.

| $C_{3v}$ | E | $2C_3$ | $3\sigma$ |
|----------|---|--------|-----------|
| $A_1$ | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | -1 |
| E | 2 | -1 | 0 |
| $\Gamma_a$ | 5 | 2 | -1 |
| $\Gamma_b$ | 7 | 1 | -1 |

5. Find the symmetries of rotational vectors $R_x$ and $R_z$ in $C_{2h}$ point group.

6. What is inverse transformation procedure?

7. Explain what is meant by a trial function?

8. What is the major difference between MOT and VBT in considering the electronic arrangement of molecules?

9. Calculate the electron densities on the carbons in allyl anion.

10. 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.

11. (i) What are the rules to be obeyed for a set of elements to form a mathematical group? (ii) Show that all integers from $-\infty$ to $+\infty$ through zero form a mathematical group.

12. What meaning is implied in the Mulliken symbols $A_g$, $B_u$ and Bg in $C_{2h}$ point group?

13. Sketch the normal modes of ammonia molecule. Depict the transformation of these normal modes under each symmetry operation and assign symmetries to each normal mode.

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

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

16. State the variation theorem. Explain in general the LCAO method for the combination of two AOs.

**(4 × 3 = 12 Weightage)**

## Section C
Answer any *two* questions. Each question carries 5 weightage.

17. Sate Great Orthogonality Theorem. What are its consequences? Using this derive the $C_{4V}$ character table.

18. By fixing three cartesian coordinates on each atom, find out the symmetries of vibrational modes of trans-$N_2F_2$. Find IR and Raman activities of fundamental vibrational modes and prove the rule of mutual exclusion.

19. Using projection operator method construct MO for $C_3H_3{}^+$

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

**(2 × 5 = 10 Weightage)**

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