

D 122468

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Name.....

Reg. No.....

**SECOND SEMESTER M.Sc. DEGREE REGULAR/SUPPLEMENTARY  
EXAMINATION, APRIL 2025**

(CBCSS)

Chemistry

CHE2C05—GROUP THEORY AND CHEMICAL BONDING

(2019 Admission onwards)

Time : Three Hours

Maximum : 30 Weightage

**Section A**

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

1. Assign Schoenflies symbol of point group for :  
(a)  $\text{CH}_2\text{Cl}_2$ . (b) Cyclohexane (chair form),
2. Generate  $3 \times 3$  matrices for :  
(a)  $C_3$ . (b)  $S_3$ .
3. Distinguish between degenerate and nondegenerate representations with examples.
4. State rules for assigning Mulliken's symbol for symmetry species.
5. You are given  $\int_{-a}^{+a} x^3 dx$ . Predict whether it is a vanishing integral or not. Justify.
6. State Laporte selection rules for electronic transitions.
7. Write projection operator  $\hat{P}_{A_1}$  for  $A_1$  symmetry under  $C_{2v}$  point group.
8. Arrange  $\text{O}_2$ ,  $\text{O}_2^+$  and  $\text{O}_2^-$  in the increasing order of stability. Justify your answer.

**Turn over**

9. Write spectroscopic term symbol for :
- (a)  $C_2$ . (b)  $O_2$ .
10. The energy of  $\pi(\rho_i)$  molecular orbitals of benzene are  $\alpha+2\beta$ ,  $\alpha+\beta$ ,  $\alpha+\beta$ ,  $\alpha-\beta$ ,  $\alpha-\beta$  and  $\alpha-2\beta$ . Find the delocalization energy.

(8 × 1 = 8 weightage)

**Section B***Answer any six questions.**Each question carries a weightage of 2.*

11. List the symmetry elements and operators associated with  $D_{3h}$  point group. Classify them into different classes of operations.
12. Taking the positional coordinates of all atoms of cis butadiene ( $C_{2v}$ ) generate a reducible representation (Characters only).
13. Derive  $C_{4v}$  characters table.
14. Predict IR and Raman active vibrations of  $NH_3$ . Use  $C_{3v}$  character table :

| $C_{3v}$ | E | $2\rho_3$ | $3\sigma_v$ |              |                         |
|----------|---|-----------|-------------|--------------|-------------------------|
| $A_1$    | 1 | 1         | 1           | $z$          | $x^2+y^2, z^2$          |
| $A_2$    | 1 | 1         | -1          | $R_z$        |                         |
| E        | 2 | -1        | 0           | $(x, y)$     |                         |
|          |   |           |             | $(R_x, E_y)$ | $(x^2-y^2, xy)(xz, yz)$ |

15. Find the molecular orbitals of  $H_2O$ . Use  $C_{2v}$  character table :

| $C_{2v}$ | E | $C_2$ | $\sigma_{vz}$ | $\sigma'_{vy}$ |          |                 |
|----------|---|-------|---------------|----------------|----------|-----------------|
| $A_1$    | 1 | 1     | 1             | 1              | $z$      | $x^2, y^2, z^2$ |
| $A_2$    | 1 | 1     | -1            | -1             | $R_z$    |                 |
| $B_1$    | 1 | -1    | 1             | -1             | $x, R_y$ | $xz$            |
| $B_2$    | 1 | -1    | -1            | 1              | $y, R_x$ | $yz$            |

16. With the help of correlation diagram explain noncrossing rule.
17. Find  $\pi(\rho_i)$  molecular orbitals of cyclo propenyl cation  $(C_3H_3)^+$ . Use  $C_3$  or  $D_3h$  character table :

| $C_3$ | E | $C_3$        | $C_3^2$      |              |                                                         |
|-------|---|--------------|--------------|--------------|---------------------------------------------------------|
| A     | 1 | 1            | 1            | $z, R_z$     | $x^2, y^2, z^2$                                         |
| E     | 1 | $\epsilon$   | $\epsilon^*$ | $(x, y)$     | $\epsilon = e^{i(2\pi/3)}$<br>$(x^2 - y^2, xy)(xz, yz)$ |
|       | 1 | $\epsilon^*$ | $\epsilon$   | $(R_x, R_y)$ |                                                         |

18. Find the hybridized orbitals of C in  $CH_4$  from quantum mechanical approach.  
(6 × 2 = 12 weightage)

### Section C

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

19. Find hybridized orbitals of B in  $BF_3$ . Use  $D_3h$  character table :

| $D_3h$  | E | $2C_3$ | $3C_2$ | $\sigma_h$ | $2S_3$ | $3\sigma_v$ |                            |
|---------|---|--------|--------|------------|--------|-------------|----------------------------|
| $A_1'$  | 1 | 1      | 1      | 1          | 1      | 1           | $x^2 + y^2, z^2$           |
| $A_2'$  | 1 | 1      | -1     | 1          | 1      | -1          | $R_z$                      |
| $E'$    | 2 | -1     | 0      | 2          | -1     | 0           | $(x, y)$ $(x^2 - y^2, xy)$ |
| $A_1''$ | 1 | 1      | 1      | -1         | -1     | -1          |                            |
| $A_2''$ | 1 | 1      | -1     | -1         | -1     | 1           | $z$                        |
| $E''$   | 2 | -1     | 0      | -2         | 1      | 0           | $(R_x, R_y)$ $(xz, yz)$    |

Turn over

20. Briefly discuss MO theory of bonding as applied to  $\text{H}_2^+$ .
21. Find the energy of  $\pi(\rho_i)$  molecular orbitals of butachene using HMO method. Also find any one of the  $\pi$  molecular orbitals.
22. Discuss briefly :
- (a) Block diagonalization.
  - (b) Frost Hückel circle mnemonic device.

(2 × 5 = 10 weightage)