Name:

Enrolment No:



UPES

End Semester Examination, December 2024

Course: Fundamentals of Group theory Program: B.Sc. (H) Chemistry by Research Course Code: CHEM4012 Semester: VII Time : 03 hrs. Max. Marks: 100

Instructions:

- 1. Write your enrolment number on the top left of the question paper.
- 2. Do not write anything else on the question paper except your enrolment number.
- 3. Attempt all parts of a question at one place only.
- 4. Internal choice is given for question number 9 of Section B and question number 11 of Section C only.
- 5. Use Character Table wherever required.

SECTION A

| | (5Qx4M=20Marks) | | |
|--------|---|-------|-----|
| S. No. | | Marks | СО |
| Q 1 | Discuss postulates of the Great orthogonality theorem. | 4 | CO1 |
| Q 2 | Determine r_{3N} for the following molecules: (a) $H_2O(C_{2v})$ (b) POCl ₃ (C_{3v}) | 4 | CO2 |
| Q 3 | Assign the point group of the following compounds: (a) BrF ₅ (b) SO ₂ | 4 | CO2 |
| Q 4 | Elaborate different types of symmetry elements present in XeF ₄ . | 4 | CO3 |
| Q 5 | Explain the following with examples: (i) Plane of symmetry (ii) Centre of symmetry | 4 | CO1 |
| | SECTION B | | |
| | (4Qx10M= 40 Marks) | | |
| Q 6 | Mention the irreducible components of the following reducible representations (use the character tables): (a) D_{3d} (b) C_{4v} | 10 | CO3 |
| Q 7 | Deduce the matrix representation for the identity rotational operation and reflectional operation, rotational–reflectional operation and inversion. | 10 | CO3 |
| Q 8 | Elaborate all the forbidden transition in D_{4h} and C_{4v} . | 10 | CO4 |

| Q 9 | Construct the character table for C_{3v} point group. | | | | |
|------|---|-------|-----|--|--|
| | OR | 10 | CO3 | | |
| | How are the irreducible representation symbolized? Write the reduction | | | | |
| | formula. Also, explain two examples for irreducible representation? | | | | |
| | SECTION-C | | | | |
| | (2Qx20M=40 Marks) | | | | |
| Q 10 | (a) Explain IR and Raman active mode in CH _{4.} | | | | |
| | (b) Consider an octahedral molecule XY ₆ whose point group is O _h . | 10+10 | CO4 | | |
| | Prove the irreducible representation of O_h is $\Gamma = A_{1g} + E_g + T_{1u}$. | | | | |
| Q 11 | (a) Explain elements of symmetry and symmetry operations. | 20 | | | |
| | (b) Find the irreducible components of the representations generated | | | | |
| | by a set of five d-orbitals in environments of T_d . | | 001 | | |
| | OR | | CO3 | | |
| | Construct SALCs corresponding to bond stretches, and in- and out-of- | | | | |
| | plane bending modes for $NH_3(C_{3v})$. | | | | |