Roll No. $\square$ Total No. of Pages: 02
Total No. of Questions : 09

## M.Sc.(Chemistry) (2015 to 2017) (Sem.-2) SYMMETRY AND GROUP THEORY <br> Subject Code : MSCH-202 <br> M.Code : 71663

Time : 3 Hrs.
Max. Marks : 100

## INSTRUCTIONS TO CANDIDATES :

1. Attempt any FIVE questions in all, including question no. 1 which is compulsory and selecting one each from units I-IV
2. Answer briefly :
$10 \times 2=20$
a. Define point group and space group.
b. What kind of improper rotation axis is present in ethane molecule?
c. Write any two important rules for the great orthogonality theorem.
d. Write all the symmetry elements present in $\mathrm{CCl}_{4}$ molecule.
e. What is the difference between proper and improper rotation axis?
f. What is the point group of ethylene molecule? How its point group is changed on dimerization?
g. Write the irreducible representation formed by the $\left[\mathrm{Ni}(\mathrm{CN})_{4}\right]^{2-}$.
h. How d-orbital split in octahedral environment according to the symmetry?
i. What does the symbol S, P, D and F stands for in Free Ion terms?
j. What do you mean by the mulliken symbol $\mathrm{T}_{\mathrm{lg}}$ and $\mathrm{E}_{\mathrm{u}}$ in the character table?

## UNIT-I

2. a. Consider the following sequential structural changes $(\mathrm{I} \rightarrow \mathrm{II} \rightarrow \mathrm{III})$. For each series indicate :
(i) Point group of each structure 5
(ii) The specific symmetry elements lost or gained in the transition $\mathrm{I} \rightarrow$ II.

I

II

III

FIG.
b. For the following molecules, sketch all the symmetry elements and list all the symmetry operations associated with each symmetry element :
i) $\mathrm{CHCl}_{3}$ 5
ii) $\mathrm{PF}_{5}$
3. a. Take the example of ethane molecule and sketch the proper and improper rotation axis present in the molecule.
b. What is the point group of (i) 1,2-Dichloroethane, (ii) cyclobutadiene and (iii) $\mathrm{PF}_{5}$ ? Write all the symmetry elements present in the molecules. 10

## UNIT-II

4. a. Construct the character table for the $\mathrm{CHCl}_{3}$ molecule having point group $\mathrm{C}_{3 \mathrm{v}}$. 10
b. What are the important rules for irreducible representation and their characters? Verify each rule by taking example of HCHO molecule.
5. a. Describe the relationship between reducible and irreducible representations by taking the example of $\mathrm{MX}_{4}$ type of molecule.
b. Write the matrix notations for the geometric transformation of symmetry element, E, $\mathrm{i}, \sigma_{v}$ and $\mathrm{C}_{2}$.

## UNIT-III

6. a. Write the symmetry adapted linear combination belongs to $\mathrm{C}_{4} \mathrm{H}_{4}$ molecule.
b. What is the symmetry based selection rules for cyclization reactions? Explain with the help of suitable example.
7. a. Construct the irreducible representation formed by the $A B_{3}$ type of trigonal planar molecule. Also calculate the SALCs on atom B.10
b. Draw the molecular orbitals for the $\sigma$-bonding in square planar $\mathrm{AB}_{4}$ molecule. 10

## UNIT IV

8. a. Draw the correlation diagram for a $\mathrm{d}^{2}$ ion in an tetrahedral environment.
b. Discuss the splitting of free ion terms ( ${ }^{1} \mathrm{~S},{ }^{1} \mathrm{G},{ }^{3} \mathrm{P}$ ) of $\mathrm{d}^{2}$ ion in $\mathrm{D}_{4 \mathrm{~h}}$ and $\mathrm{T}_{\mathrm{d}}$ point groups.
9. a. Construct the energy level diagram of e and $t_{2}$ orbitals resulting from splitting of dorbital in octahedral environment.
b. What is orbital and spin degeneracy? Explain by taking example of $\mathrm{e}_{\mathrm{g}}$ configuration.

NOTE : Disclosure of Identity by writing Mobile No. or Making of passing request on any page of Answer Sheet will lead to UMC against the Student.

