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Total No. of Questions : 09

M.Sc.(Chemistry) (2015 to 2017) (Sem.–2)

SYMMETRY AND GROUP THEORY

Subject Code : MSCH-202

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**

1. Answer briefly : **10×2=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 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 $[Ni(CN)_4]^{2-}$.

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 T_{1g} and E_u in the character table?

UNIT-I

2. a. Consider the following sequential structural changes (I → II → III). For each series indicate :

(i) Point group of each structure 5

(ii) The specific symmetry elements lost or gained in the transition I → II. 5

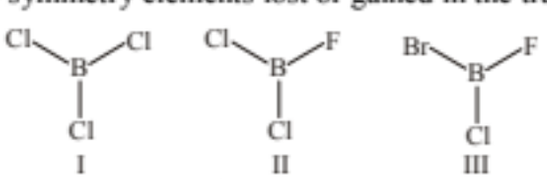

FIG.

b. For the following molecules, sketch all the symmetry elements and list all the symmetry operations associated with each symmetry element :

i) $CHCl_3$ 5

ii) PF_5 5

3. a. Take the example of ethane molecule and sketch the proper and improper rotation axis present in the molecule. 10

b. What is the point group of (i) 1,2-Dichloroethane, (ii) cyclobutadiene and (iii) PF_5? Write all the symmetry elements present in the molecules. 10

UNIT-II

4. a. Construct the character table for the $CHCl_3$ molecule having point group C_{3v}. 10

b. What are the important rules for irreducible representation and their characters? Verify each rule by taking example of HCHO molecule. 10

5. a. Describe the relationship between reducible and irreducible representations by taking the example of MX_4 type of molecule. 10

b. Write the matrix notations for the geometric transformation of symmetry element, E, i, σ_v and C_2. 10

UNIT-III

6. a. Write the symmetry adapted linear combination belongs to C_4H_4 molecule. 10

b. What is the symmetry based selection rules for cyclization reactions? Explain with the help of suitable example. 10

7. a. Construct the irreducible representation formed by the AB_3 type of trigonal planar molecule. Also calculate the SALCs on atom B. 10

b. Draw the molecular orbitals for the σ-bonding in square planar AB_4 molecule. 10

UNIT IV

8. a. Draw the correlation diagram for a d^2 ion in an tetrahedral environment. 10

b. Discuss the splitting of free ion terms (^1S, ^1G, ^3P) of d^2 ion in D_{4h} and T_d point groups. 10

9. a. Construct the energy level diagram of e and t_2 orbitals resulting from splitting of d-orbital in octahedral environment. 10

b. What is orbital and spin degeneracy? Explain by taking example of e_g configuration. 10

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.