Birla Institute of Technology & Science, Pilani
Hyderabad Campus

AGSRD

FIRST SEMESTER 2019-2020

Course Handout (Part - II)

Date: 03/08/2019

Course No. : CHEM G541
Course Title : Chemical Applications of Group Theory
Instructor-in-charge : **Balaji Gopalan**

Scope and Objective: Symmetry and application of the group theoretical methods in various chemical instances in Chemical Bonding, Hybridization, Molecular Orbital Theory, Normal modes, to molecular spectroscopy, Selection rules in spectroscopy and to predict the Infrared and Raman activity of molecular vibrations etc. will be discussed at an advanced level. Briefly, it would touch upon the following:

Groups, subgroups and classes: definitions and theorems; molecular symmetry and symmetry groups; representation of groups; character tables; wave functions as bases for irreducible representations; direct product; symmetry adapted linear combinations; symmetry in molecular orbital theory; hybrid orbitals; molecular orbitals of metal sandwich com- pounds; ligand field theory; molecular vibrations; space groups.

Text Book (T):

"Chemical applications of Group theory" F. A. Cotton, Third Ed. Wiley (1990).

Reference Books:

R1 'Quantum Chemistry', Ira N Levine, 6th edition, Pearson Education Inc. (2009).

R2. "Molecular symmetry and Group theory" Robert L Carter, Wiley (1998).

Course Plan:

Lec. No.	Learning Objectives	Topics to be covered	Ref to text
Molecular Symmetry and Symmetry group			
1-5	Symmetry operations and Group theory	Symmetry elements, Classes of operation, Point groups and its classification, Application of symmetry operations, dipole moment and optical activity	T 3.1 - 3.14, R1 Chapter 12 R2 1.5 to1.7
Representation of groups			

6-14	Group multiplication table, sub groups, Representations of groups, Equivalent and reducible representation, irreducible representation and quantum mechanics, Properties of characters of representation.	Construction of multiplication and character tables, Irreducible and reducible representations, transformation operators, Great Orthogonality Theorem, Character tables and their constructions, Hamiltonian operator under transformation, direct product representation, vanishing integrals.	T 4.1 - 4.5 T 5.1 - 5.3 R2 Chapter 2 (2.1 to 2.5) Discussion notes
15-20	Symmetry and hybrid orbitals	Determination of symmetry of hybrid orbitals-general discussion, Symmetry of hybridization of various molecules	T Chapter 6
21-26	Symmetry and chemical bonding	Symmetry adopted bases (SALCs), degeneracy, Projection operators	T 6.1-6.3, R2 4.3, 5.1-5.2
27-31	Molecular vibrations, Determination of symmetry of vibrational modes	Reducible representations for the normal modes, general discussion and worked examples	T1 10.1-10.8 Discussion notes
32-36	Applications in Molecular orbital Theory	Transformation properties of atomic orbitals, Construction of ligand group orbitals for molecules, examples AB_4 tetrahedral, AB_2 bent and AB_2 linear, AB_3 planar and pyramidal molecules	7.1-7.8 8.1-8.8
37-42	Applications in Spectroscopy;	Normal coordinates, vibrational levels, Selection rules, Mutual exclusion Principle, IR and Raman activity of molecules, Polarisation of Raman linesSelection Rules for electronic transitions.	10.1-10.8

Evaluation Scheme:

Component	Duration	Weightage(%)	Nature	Date & Time
Assignments	30 min	25	Open	
Presentation/Seminar	30 min	15	Open	
Mid Sem Evaluation		20	Closed book	
Final assessment	3 hrs	40	Closed book	

Chamber Consultation Hour: Will be announced later in the class and also will be displayed in the notice board.

Notices concerning the course will be displayed only in the Chemistry Dept. Notice Board.

Academic Integrity Policy: It is expected that in compliance with institute rules and regulations, academic integrity should be adhered to in all the evaluation components. Malpractice in any form will have serious implications.

Instructor in Charge
Balaji Gopalan