INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH, MOHALI

SECOND SEMESTER 2009-2010

CHM304: SYMMETRY IN CHEMISTRY

Course Handout

Date: 06.01.2010

Course No. **: CHM304**
Course Title **: Symmetry in Chemistry**
Instructor **: Angshuman Roy Choudhury**

1. **Course Description:** The course will concentrate in the chemical applications of group theory. Basic concepts of group theory molecular and crystallographic symmetry will be covered with suitable applications of group theory.

2. **Scope & Objective of the Course:** Definitions and theorems of group theory, molecular symmetry, symmetry groups, and representations of groups will be discussed in detail. The concept will be elaborated with suitable applications in MO theory or organic, inorganic and organometallic compounds, ligand field theory and molecular vibrations. Basic crystallographic symmetry and space group concept will also be covered.

3. **Text Book(T):** (1) F. A. Cotton, Chemical Applications of Group Theory, Indian Edition, 3rd Ed, Wiley-India, Noida, 2003,

4. **Reference Book(R):** (1) D. M. Bishop, Group Theory and Chemistry, 1st Ed, Dover Publications, New York, 1993; (2) H. H. Jaffe, M. Orchin, Symmetry in Chemistry, 1st Ed, Dover Publications, New York, 2002.

3. **Course Plan:**

Lec. Nos.	Learning Objectives	Topics to be Covered	Book/Chapter Number
1-2	Introduction and definitions and theorems of group theory	Defining properties of groups, group multiplication tables, group orders, cyclic groups, subgroups, classes and theorems	T1, 2.1-2.4
3-7	Molecular symmetry and symmetry groups	Symmetry elements and operations, plane of symmetry, inversion centers, proper and improper axes of rotation, products of symmetry operations, equivalent symmetry elements and points, symmetry elements and optical isomerism, symmetry point groups, platonic solids and their point group symmetry, classes of symmetry operations, illustrative examples.	T1, 3.1-3.14
8-12	Representation of groups	Matrices and vectors, matrix multiplication, matrix notation or geometric transformations, vectors and their scalar products, representation of groups, the Great Orthogonality Theorem" and its consequences, character tables, representation of cyclic groups.	T1/4.1-4.5
13-14	Group theory and quantum mechanics	Wave functions as bases for irreproducible representations, direct product and its use, spectral transition probabilities	T1/5.1-5.3
15-19	MO Theory and its application in organic chemistry	Introduction, LCAO approximation, Hückel approximation, energy level diagrams, Hund's rule and the Exclusion principle, bonding character of orbital, carbo-cyclic systems, aromaticity (4n+2 rule).	T1/7.1-7.3
20-21		Symmetry bases selection rules for cyclization reaction	T1/7.8

22-25	MO Theory for inorganic and organometallic compounds	Introduction, transformation properties of AOs, MO for σ bonding in AB_n (n = 3-6) molecules, hybrid orbital, MO for π bonding in AB_n (n = 4, 6) molecules, cage and cluster compounds, metal sandwich compounds.	T1/8.1-8.8
26-30	Ligand field theory	Introduction, free atoms and ions, term symbols, quantum numbers for any electron atoms, splitting of levels and terms, construction of energy level diagrams, Hole Formalism, Tanabe-Sugano diagram, spectral and magnetic properties of complexes, crystal field theory, selection rules and polarizations, double groups,	T1/9.1-9.7
31-35	Molecular vibrations	Introduction, symmetry and normal vibrations, determination of symmetry of the normal modes, selection rules for fundamental vibrational transitions, illustrative examples, exclusion rules, Fermi Resonance, Solid State effects, Site symmetry approximations, correlation field approximation,	T1/10.1-10.3, 10.6-10.8
36-40	Crystallographic symmetry	Introduction, concept of lattice and symmetry in 2D and 3D, crystal symmetry and crystallographic point groups, point group representations, inter-relation between lattice symmetry, crystal symmetry and diffraction symmetry, additional symmetry elements-screw axis, glide plane, standard symbols for symmetry elements, 230 space groups and their representation in 2D.	T1/11.1-11.8

4. **Evaluation Scheme:**

EC NO.	Evaluation Component	Duration	Marks	Weightage(%)	Date Time Venue	Nature of Component
1.	Mid-sem I	1 hr.	40	20		Closed Book
2.	Mid-sem II	1 hr.	40	20		Closed Book
3.	Quiz	In class	40	10		Closed Book
4.	Final Exam.	3 hrs	80	50		Closed Book

5. **Chamber Consultation hours:** To be announced in the class.
6. **Make-up Policy:** Make-up will be granted following institute rules.
7. **Notices:** Relevant notices regarding the course will be displayed on Notice Board.

Instructor
CHM304