FIRST SEMESTER 2015-16

Course Handout Part II

Date: -3/08/2015

In addition to part -I (General Handout for all courses appended to the timetable) this portion gives further specific details regarding the course.

Course No. **: CHEM G541**

Course Title **: Chemical Applications of Group Theory**

Instructor-in-charge **: Ram Kinkiar Roy**

1. Course Description: 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 compounds; ligand field theory; molecular vibrations; space groups.

Scope and Objective of the Course:

The course aims to show how the abstract concept of Group and the mathematical developments based on this concept are useful in explaining the symmetry aspects of molecules and crystals. Further it will be shown how a systematic understanding of symmetry simplifies and saves time in the theoretical quantum chemical calculations.

2. Text and Reference Books:

Text Book(s):

T1. Cotton F.A., "**Chemical Applications of Group Theory**", 3rd ed., John Wiley and Sons, New York (2004).

Reference Book(s):

R1. Huheey J. E., and others, " **Inorganic Chemistry**", Indian Adaptation, Pearson Education South Asia, New Delhi (2006) (From the original 4th ed., Pearson Education, New York (1993))

3. Course Plan:

Lec. No.	Topics to be covered	Learning Objectives	Ref: Chap./Sec.#(Book)
1-3	Basic concepts of groups	Abstract Algebraic Groups; Concepts such as subgroups, classes;	Ch. 2 (T1)
4-6	Molecular symmetry	Symmetry elements and symmetry operations	3.1-3.10 (T1)

7-11	Point Groups and Character Tables	Symmetry operations forming a point group; Great orthogonality theorem; representation of group elements; construction and usage of character tables	3.11-3.15, Ch. 4(T1)
12-13	Uses of point group symmetry	Relevance of symmetry in optical activity, dipole moments etc.	Ch. 3(T1) Class Notes
14-17	Symmetry Adapted Linear Combinations	Projection Operators and simple examples in σ and π systems	Ch. 6 (T1)
18-20	Group Theory and Quantum Mechanics	Direct Product and its utility; spectral transition probabilities	Ch 5(T1)
21-24	MO Theory – Organic systems	Symmetry factoring of secular equations; electronic excitations; selection rules for cylcisation.	Ch 7(T1)
25-28	MO Theory – Inorganic systems	Details of σ bonding and hybridizations; Cage , cluster and sandwich compounds	Ch 8(T1
29-32	Ligand Field Theory	Splitting of levels in a geometry; selection rules; double groups; TS diagrams	Ch. 9(T1)
33-36	Molecular vibrations	Normal modes, F and G Matrix methods, Selection Rules	Ch. 10(T1)
37-40	Crystallographic symmetry	Lattice, Crystallographic Point Groups, glide planes and screw axis, space groups	Ch 11(T1)

4. **Evaluation Components:**

Components	Weightage(%)	Dates	Type
Mid-Sem. Test Closed Book	30%	9/10 10:00 - 11:30 AM	
Assignments /Seminars Quizzes	30%	Continuous	Partly Closed Book
Comprehensive Examination 40%		10/12 AN	Partly Open Book

Home Assignments: Assignments will be given periodically to supplement the material discussed in class. See Evaluation Scheme above for weightage. These will include problem sets and certain literature based exercises, some of which may be of routine, and others of advanced nature. The problem sets and other exercises will be discussed in the class or chamber consultation hour. Students will also be asked to solve some problem(s) during the class hour for evaluation. Students will also have to deliver seminars on some topics.

5. **Chamber Consultation Hour:** Monday 10th Hr. (5-6 PM); 3144-A

Instructor-in-charge
CHEM G541