

MU'TAH UNIVERSITY
DEPARTMENT OF CHEMISTRY
CHEMICAL APPLICATIONS OF GROUP THEORY "CHEM 721"
FALL SEMESTER 2017/2018

Instructor: *Professor Dr. Arab Qaseer*
Lectures' times: Sunday (2.00 – 5.00 PM)
Credit hours: 3
Text book: Chemical Applications of Group Theory by F.A. Cotton, John Wiley and Sons, Inc., 3rd Ed., 1990.

Syllabus:-

Part I. Principles

Chapter 2. DEFINITIONS AND THEOREMS OF GROUP THEORY

Properties of a group; examples of groups; subgroups, classes.

Chapter 3. MOLECULAR SYMMETRY AND THE SYMMETRY GROUPS

Symmetry elements and operations; symmetry planes and reflections; the inversion center; proper axes and proper rotations; improper axes and improper rotations; products of symmetry operations; symmetry elements and optical isomerism; classes of symmetry operations; procedure for symmetry classification of molecules, and illustrative examples.

Chapter 4. REPRESENTATIONS OF GROUPS

Comments on matrices and vectors; representations of groups; character tables; representations for cyclic group, worked examples.

Chapter 5. GROUP THEORY AND QUANTUM MECHANICS

Wave functions as bases for irreducible representations; the direct product; nonzero matrix elements, worked examples.

Chapter 6. SYMMETRY - ADAPTED LINEAR COMBINATIONS (SALCS)

Derivation of projection operators, how to construct SALCs, and exercises.

Part II. Applications

Chapter 7. MOLECULAR ORBITAL THEORY AND ITS APPLICATIONS IN ORGANIC CHEMISTRY

Secular Equations; carbocyclic systems; LCAO-MO π Bonding, a worked example Naphthalene; electronic excitations of Naphthalene; three-center bonding and selection rules for cyclization reactions.

Chapter 8. MOLECULAR ORBITAL THEORY INORGANIC AND ORGANOMETALLIC COMPOUNDS

MO for σ bonding in AB_n molecules: T_d (AB_4) case; hybrid orbitals; MO for π bonding in AB_n molecules, and MO for metal sandwich compounds.

Chapter 9. LIGAND FIELD THEORY

Electronic structures of free atoms and ions; construction of energy level diagrams; estimation of orbital energies; selection rules and polarizations.

Chapter 10. MOLECULAR VIBRATIONS

The symmetry of normal vibrations; determining the symmetry types of the normal modes; selection rules for fundamental vibrational transitions; illustrative examples.

Exams and Evaluations

Exam	Date	Evaluation
First Exam	Week 7	30%
Second Exam	Week 12	30%
Final Exam	As Described by the Registrar	40%
Total		100%

GOOD LUCK