



Jordan University of Science and Technology
Faculty of Science & Arts
Chemistry Department

CHEM721 Physicochemical Methods In Inorganic Chemistry

First Semester 2017-2018

Course Catalog

3 Credit Hours. The general objective of this course aims to make the students fully acquainted with the theories and applications of group theory, molecular symmetry and its applications as to chemical bonding and molecular spectroscopy. The course starts with definitions and properties of groups, subgroups, classes, and cyclic groups. Once this is covered the course will deal with symmetry elements and point groups, direct product of symmetry elements and multiplication tables of a variety of groups, Mulliken Symbols with different notations. The second subject in this course deals mainly with combination of symmetry considerations and hybridization schemes for π -type orbitals in different molecules. Next, the subject of projection operator will be covered and also the application of this concept to symmetry adapted linear combination of atomic orbitals (SALCAO-concept). Both π and σ orbital combination will be covered employing the projection operator concept. The second part deals with Huckle approximation theory which is employed to solve for the energy of different levels for different combinations of cyclic conjugated and linear conjugated π -systems and the determination of resonance stabilization energy in these molecules, radicals, or ions. The third part will deal with normal modes of vibrations in different molecules and methods of determination of these modes by using symmetry considerations to determine which of these modes are IR-active, Raman-active or both. The last part of this course will cover ligand field theory, Russell-Saunders term symbols and microstates. Finally, the principles and selection rules in vibrational and electronic transition spectroscopies will be discussed in details

Text Book

Title	Chemical Applications of Group Theory
Author(s)	F. A. Cotton
Edition	3rd Edition
Short Name	Text book
Other Information	1990, J.Wiley & Sons

Course References

Instructor	
Name	Prof. Khalil Asali
Office Location	N4L0

Office Hours	Sun : 11:00 - 12:30 Mon : 10:00 - 13:00 Tue : 13:30 - 14:30 Thu : 09:30 - 10:30
Email	asali@just.edu.jo

Class Schedule & Room
Section 1: Lecture Time: Sun, Tue : 15:00 - 16:30 Room: M1305

Tentative List of Topics Covered		
Weeks	Topic	References
Week 1	Definition and Theorems of Group Theory	Chapter 2 From Text book
Week 2	1. 1. What do we mean by a symmetry element. 2. 2. Types of symmetry elements; definition with specific examples: a. 3. Plane of symmetry σ b. Center of inversion i c. Proper axis of symmetry C_n d. 4. Improper axis of symmetry S_n . 3. 5. Examples of determination of symmetry elements in some molecules such as H ₂ O, NH ₃ , CH ₄ , BH ₃ , octahedral molecules AB ₆ .	Chapter 3 From Text book
Week 3	1. Direct products of symmetry operations 2. 2. Commutation and noncommutation of some symmetry operation $AB=BA$, or $AB \neq BA$ concepts. Eq 3. equivalent and nonequivalent atoms from symmetry point of view. Sy 4. Systematic determination of point groups. 5. Illustration of point group of different molecules including C _{2v} , C _{3v} , C _{4v} , T _d , D _{3h} , D _{4h} 6. 6. Classes of symmetry operations	Chapter 3 From Text book
Weeks 4, 5	Representation of Groups	Chapter 4 From Text book
Week 6	1. General transformation properties of atomic orbitals. 2. Hybridization scheme for p -type orbitals in tetrahedral AB ₄ . 3. Hybridization scheme for p -orbitals in planar AB ₃ , trigonal bipyramidal AB ₅ and octahedral AB ₆ molecules.	Chapter 8 From Text book
Week 7	1. General introduction to symmetry-adapted linear combination of atomic orbitals. 2. 2. The projection operator and the method and application of this operator for to different symmetry operations. 3. 3. Solved examples on projection operators in some functions under some point groups such as C _{3v} , C _{2v} and D _{3h} point group. 4. p -orbitals for cyclopropenyl group under D _{3h} S symmetry employing the projection operator. 5. 5. Method of using the cyclic group C ₃ to derive the different p - p -combination functions in C ₃ H ₃ group. 6. Normalization of the obtained wave functions with stress on the orthogonality concept.	Chapter 6 From Text book
Week 8	1. SALCOAO in benzene molecule using the projection operator on one p of the six equivalent p 's. 2. Normalization and profiles of the six combination functions obtained. 3. Definition what is meant by the Hamiltonian $H_{ii} = ?$ and that $H_{ij} = ?$ the overlap integral and how we get the proper determinant to solve the different coefficients in the combined wave-functions. 4. An introduction to Huckle approximation theory employed to solve for the different energy levels for different combinations.	Chapter 7 and 6 From Text book

Weeks 9, 10	1. 1. Carbocyclic systems: SALCAO-MO and Energy levels in benzene under D _{6h} point group. 2. 2. Estimation of delocalization energy (resonance) energy in benzene in units of ?. 3. 3. Estimation of the energy of the first HOMO to LUMO transition in benzene. 4. 4. Estimation of the energy of the first HOMO to LUMO transition in benzene. 5. 5. The molecule tetramethylenecyclobutane under D _{4h} point group. 6. Derivation of the kind of overlap in two sets of the carbon p _z orbitals, each set consists of four equivalent p _z orbitals. 1. 7. Determination of the energy, in units of ? for the eight MO's obtained. 2. 8. Determination of the delocalization energy in this molecule. 3. 9. Calculation of the energy of the first electronic transition between the HOMO-LUMO orbitals in this molecule.	Chapter 7 & 5 From Text book
Week 11	Molecular Vibrations	Chapter 10 From Text book
Week 12	1. Wave functions and quantum numbers for a single electron. 2. Quantum numbers for many electrons. Russell-Saunders term symbols. Orbital-orbital coupling and spin multiplicity concept, ?l and ?s. 3. Russell-Saunders term symbols and microstates for d ₁ and d ₂ electrons in free ions. 4. Determination of spin multiplicity for every term obtained in (1). 5. Determination of characters of the five-dimensional matrix obtained by rotation by an angle ? to get the ?(C?) reducible representation and then reduce it to the corresponding irreducible representations. 6. Construction of energy level diagram for d ₂ in free ion. 7. Splitting of the different states under very weak interaction with determination of spin multiplicity for every state.	Chapter 9 From Text book
Week 13	1. 1. Electronic distribution in d-split levels of two electrons under ? interaction and then relaxation of interaction under very strong interaction. 2. 2. Applying Hoffman-Woodward rules for spin-noncrossing rule to obtain the final correlation diagram for d ₂ system. 3. 3. Determination of the type of possible electronic transitions from the ground state to some other excited states taking into consideration some rules and restrictions. 4. 4. Method of descending symmetry : Oh ? D _{4h} 5. 5. Descending symmetry in general Oh ? C _{4v} ? D _{4h} ? C _{2v} . 6. 6. General schemes for reduced symmetry.	Chapter 9 From Text book
Week 14	1. Selection rules in electronic transition spectroscopy. 2. Laporte-rule for electronic transition restriction, in molecules which have a center of symmetry i such as Oh and D _{4h} symmetries; d-d forbidden, g-g forbidden transitions. 3. Spin forbidden transitions. 4. Restrictions transitions in centrosymmetric molecules in general. 5. Revision	Chapter 9 From Text book

Mapping of Course Objectives to Program Student Outcomes¹	Assessment method
Students should be able to relate symmetry considerations to some important properties of groups. [1a, 1b, 1d, 1k]	
The students will develop good understanding of the relation between symmetry and various areas of spectroscopy such as NMR, stretching frequencies, normal modes of vibrations and electronic spectroscopies. [1c, 1j]	
One of the most important outcomes of this course is that the students will be familiar with the concepts of selection rules in vibrational and electronic spectroscopies. This will be related directly to chemical application of group theory [1i]	

Relationship to Program Student Outcomes (Out of 100%)										
a	b	c	d	e	f	g	h	i	j	k
12.50	12.50	12.50	12.50					25	12.50	12.50

