بسم الله الرحمن الرحيم

جامعة آل البيت

جامعة آل البيت
دائرة ضمان الجودة والتخطيط

كلية .....العلوم.....

قسم .....الكيمياء.....

توصيف مساق....Chem 403721.....

1. معلومات مدرس المساق (Instructor)

اســـم (مدرس / منسق) المساق :	Harbi Al-Masri
الساعـــــات المكتبيـــــــــــة :	9.15-10.15 Sun-Wed
رقم المكتب والرقـــم الفرعـــــي :	
البريـــــــــد الالكترونـــــــي :	Harbi28@yahoo.com
مساعد البحث والتدريس/المشرف/الفني (إن وجد):	NA

2. وصف المساق (Course Description)

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 deals 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 **σ**- 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 **σ** and pi 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

3. بيانات المساق (Course Title)

رقم المساق: 403721	**اسم المساق:** Chemical Applications of Group Theory	**المستوى: Master**

طبيعة المساق: نظري	المتطلب السابق / المتزامن :----None---	وقت المحاضرة: 8-9.15
العام الجامعي:2021/ 2020	الفصل الدراسي:First	عدد الساعات الدراسية:3

4. أهدافالمساق (Course Objectives)

Comprehensive introduction to concepts properties of Groups and the relationship between groups and symmetry elements.	أ-
Understand the application of group theory to molecular symmetry and point groups	ب-
Develop a general understanding of symmetry and orbital hybridization.	ج-
Understand how symmetry can be employed to solve for energy levels in systems with open and cyclic conjugated π - orbitals	د-
Understand Normal modes of vibrations and the selection rules to this area of spectroscopy and the concept of electronic transitions and the selection rules in this area of spectroscopy.	

5. مخرجات التعلم (Intended Student Learning Outcomes)

(المعرفة والمهارات والكفايات)

يفترض بالطالب بعد دراسته لهذا المساق أن يكون قادرا على:

After completing the course, the student will be able to:

1. Students should be able to relate symmetry considerations to some important properties of groups.
2. The students will develop good understanding between symmetry and various areas of spectroscopy such as NMR, stretching frequencies, normal modes of vibrations and electronic spectroscopy.
3. 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

4. محتوى المساق(Course Content)

الأسبوع	الموضــوع
الأول	**1**.Definition of a group. **2**.Elements of a group **3**.Examples of groups and its general properties. **4**.Subgroups within a group. **5**.Solved examples how subgroups within a group are found. **6**.Cyclic and Abelian groups. **7**.What do we mean by a symmetry element. **8**.Types of symmetry elements; definition with specific examples: **9**.Plane of symmetry $\boldsymbol{\sigma}$ b. Center of inversion $\boldsymbol{i}$ c. Proper axis of symmetry C_n **10**.Improper axis of symmetry $\boldsymbol{S_n}$. **11**.Examples of determination of symmetry elements in some molecules such as H_2O, NH_3, CH_4, BH_3, octahedral molecules AB_6.

1. Products of symmetry operations 2. Commutation and noncommutation of some s symmetry operation AB=BA or AB≠BA ıcepts. 3. equivalent and nonequivalent atoms from symm- sy try po point of view, examples. 4. Systematic determination of point groups. lustration of point group of different molecules including C2v , C3V, C4V, Td, D3h, D4h 5. Classes of symmetry operations ıeral properties of a matrix; order of a matrix and combination of matrices with specific examples of 2x2 and 3x3 matrices. **6.** Matrix representation of different symmetry operation such as the specific matrices for proper rotation, inversion, reflection, and improper rotations. **7.** Derivation of the general matrix which represent rotation by an angle θ . Reducible and irreducible representations. **8.** The theory of orthogonality and its application in groups.	الأول
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. 1.General rules about irreducible representations and their characters. **2.** Examples and applications. Components of a character table with specific point group such as C_{3v} . **3.** Discussion and illustration of the symbols given for different irreducible representations 4.known as Mulliken Symbols with different notations; A, B, E, and T which present with different characters in various point groups. **4.** General transformation properties of atomic orbitals. 5.Hybridization scheme for σ-type orbitals in tetrahedral AB_4. **6.**Hybridization scheme for σ-orbitals in planar AB_3, trigonal bipyramidal AB_5 and octahedral $_6$ molecules. 7. SALCOAO in benzene molecule using the projection operator on one Φ of the six equivalent Φ's. 8. Normalization and profiles of the six combination functions obtained. 9. Definition what is meant by the Hamiltonian Hii = α and that Hij = β the overlap integral and how we get the proper determinant to solve the different coefficients in the combined wave-functions. 10. An introduction to Huckle approximation theory employed to solve for the different energy levels for different combinations.	الثالث + الرابع
First Exam (End of week 4; Chapters 1-3)	
1. General introduction to normal modes of vibrations. **2.** The symmetry and number of normal modes, 3n-6 rule.	الخامس

3. Matrix representation of the contribution of every symmetry operation to determine the irreducible representation for 3n normal modes. **4.** The irreducible representations for the normal modes of vibration of CO_3^{2-} , **5.** Determination of which of these representations IR active and which ones are Raman active with the help of the given character table. **6.** The irreducible representations for H_2O (C_{2V}), NH_3 (C_{3V}), and CH_4 (T_d), each under its specific point group, with determination of which of these modes are IR active and which are Raman active. **7.** Selection rules for normal modes of vibration. **8**. The symmetry of the ground state; Ψ_v^o and the excited state; Ψ_v^i for molecular vibration. 9. Conditions which should exist for a fundamental to be IR active. **10**. Specific examples on the application of selection rules	الخامس
1. **1.** Carbocyclic systems: SALCAO-MO and Energy levels in benzene under D_{6h} point group. **2.** Estimation of delocalization energy (resonance) energy in benzene in units of β. **3.** Estimation of the energy of the first HOMO toLUMO transition in benzene. **4.** Estimation of the energy of the first HOMO toLUMO transition in benzene. 5. Definition and application of local symmetry. **6.** How the local symmetry can be employed to determine the stretching frequencies in metal carbonyl complexes **7.** Solved examples on local symmetry: $\nu_{(CO)}$ for octahedral $M(CO)_6$, trigonal bipyramidal $Fe(CO)_5$, mono-, di-, and tri-, substituted octahedral metal carbonyls with special emphasis on how IR spectroscopy can be used to distinguish among some *cis* and *trans* isomers in some of these complexes. 8. Introduction to the principle of overtone formation $2\nu_i$, $2\nu_k$, and combination overtones of the type $(\nu_i + \nu_k)$. **9.** Selection rules for combination of an overtone with a fundamental. The phenomena of intensity borrowing and Fermi type resonance.	االسادس
1. The molecule tetramethylenecyclobutane under D_{4h} point group. **2.** Derivation of the kind of overlap in two sets of the carbon pπ orbitals, each set consists of r equivalent pπ orbitals. **3.** Determination of the energy, in units of β. for the eight MO's obtained. **4.** Determination of the delocalization energy in this molecule. **5.** Calculation of the energy of the first electronic transition between the HOMO-LUMO orbitals in this molecule.\ 6. Wave functions and quantum numbers for a single electron **7.** Quantum numbers for many electrons. Russell-Saunders term symbols. Orbital-orbital coupling and spin multiplicity concept, Σ*l* and Σ*s*. 8. Russell-Saunders term symbols and microstates for d^1 and d^2 electrons in free ions. **9.** Determination of spin multiplicity for every term obtained in (1). **10.** Determination of characters of the five-dimensional matrix obtained by rotation by an angle α to get the $\chi(C_\alpha)$ reducible representation and then reduce it to the corresponding irreducible representations. **11.** Construction of energy level diagram for d^2 in free ion. **12.** Splitting of the different states under very weak interaction with determination of spin multiplicity for every state.	السابع
Second Exam (End of week 7)	

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 $O_h \rightarrow C_{4v} \rightarrow D_{4h} \rightarrow C_{2v}$. 6. **6.** General schemes for reduce symmetry.	الثامن
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 D4h symmetries; d-d forbidden, g-g forbidden transitions. 3. Spin forbidden transitions. 4. Restrictions transitions in centrosymmetric molecules in general	التاسع
1. d-p mixing in centrocymmetric complexes. **2.** Vibrational-electronic; vibronic, mixing; rules and restrictions. **3.** Vibronic polarization in lower symmetry molecules. **4.** Selection rules for electronic transitions in noncentrosymmetric molecules such as tetrahedral and other molecules. **5.** Examples from experimental data on number and intensity of electronic transitions with vibronic coupling considerations.	**العاشر**

9. استراتيجيات التعليم والتعلم وطرق التقويم
(Teaching and learning Strategies and Evaluation Methods)

نوع التقويم/القياس (امتحان/عروض صفية/مناقشة/واجبات)	أنشطة التعلم	استراتيجياتالتدريس	مخرجات التعلم	ت
- Examination	- Class notes - Continuous discussion of the material - Problem sets and solutions. - Assignments	- Power point Lectures - Homeworks - Problem solving - Oral discussions - Class room participation and assignments	- Development of critical thinking and analysis - Using the lessons, examples, explanatory discussion, and analysis to demonstrate the difference. - Repetition to install the knowledge in	1

	the mind of the student. motivating and encouraging students to do their best			

1. تقييم الطلبة (Assessment)

الأساليب المستخدمة	توقيت التقييم	توزيع الدرجات لكل أسلوب
1-أعمال الفصل: (تقرير، وظائف، حضور)	خلال الفصل	10
2-امتحان تحريري أول	الأسبوع الرابع	20%
2-امتحان تحريري ثاني	الأسبوع السابع	20%
3-امتحان تحريري نهائي	أسبوع الامتحانات النهائية	50%

2. الكتاب المقرر (Text Book)

المرجع الرئيس	Chemical Applications of Group Theory
المؤلف	F. Albert. Cotton
الناشر	Wiley-Interscience.
السنة	1990
الطبعة	3th Ed.
الموقع الالكتروني للمرجع	Iwww.amazon.com/Chemical-Applications-**Group-Theory**-3rd

3. المراجع الإضافية (References)(وتشمل الكتب والبحوث المنشورة في الدوريات او المواقع الالكترونية)

M olecular Symmetry and Group Theory. Robert L. Carter, John Wiley&Sons Inc, 1998.	-1
Molecular Symmetry and Group Theory, R. L. Carter, 1988, Wiley&Sons.	-2
Symmetry: An Introduction to Group Theory and Its Applications, by Roy Mcweeny, 3rd Ed.	-3