SYLLABUS
Chem 509
Spring 2019

Group Theory: Mathematical definitions of groups and representations, applications to chemical structure and spectra, ligand field theory, chemical reactions, and selection rules.

Lectures: MWF 1:10-2:00 PM in Fulmer 225.

Instructors: Prof. Ursula Mazur (Fulmer VIF N116A) 335-5822 umazur@wsu.edu. Office hours, Wednesday 2-4 PM (tentative).

Teaching Assistant: Ms. Kristen Johnson (Fulmer 116C) kristen.johnson@wsu.edu. Office hours by appointment.


Credits: 3

Preparation: Undergraduate or basic graduate level Quantum Mechanics is recommended but not required.

Goals: The overall objective is to acquaint students with the fundamentals of symmetry and group theoretical methods and how to apply them to vibrational and electronic spectroscopy and to the study of molecular structure, bonding, and chemical reactivity.

Learning Outcomes:

- Proficiency in using concepts of molecular symmetry to identify physical properties
- Proficiency in applications of symmetry and group theory to various types of chemical systems; classification of molecules into symmetry point groups and use of character tables.
- Proficiency in constructing molecular orbitals and understand their role in determining molecular properties and reactivity
- Understanding of principles and applications of spectroscopic techniques for determination of molecular structure
- Basic understanding of solid state group theory

Topics:

- Mathematical definition of a group; symmetry operations and symmetry elements; symmetry classification of molecules – point groups, symmetry and physical properties: polarity, chirality etc.
- Combining symmetry operations: ‘group multiplication’, review of matrices, matrix representations of groups with examples
- Properties of matrix representations: similarity transforms, characters of representations, irreducible representations (IR) and symmetry species, character tables
• Reduction of representations: The Great Orthogonality Theorem; using the GOT to determine the irreducible representations spanned by a basis

• Symmetry adapted linear combinations, bonding in polyatomics, constructing molecular orbitals from SALCs, calculating and solving orbital energies and expansion coefficients

• Molecular vibrations: determining the number of vibrational normal modes, determining the symmetries of molecular motions, molecular vibrations using internal coordinates

• Spectroscopy: group theory and molecular electronic states, electronic transitions in molecules, vibrational transitions in molecules

• Morphological symmetry, crystallographic point groups, and geometric crystal classes

Lectures: Lectures should be attended regularly and students are responsible for making up the missed materials. Assignments and exams will be based primarily on lecture and reading material.

Homework: Homework assignments will be posted almost every Wednesday and will usually be due the Friday of the following week (i.e. you will have about 10 days to complete each homework) and must be turned in at the beginning of the class. The intent is to allow you a bit of flexibility so that you can budget your time accordingly. You are encouraged to work in groups. I hope that you will use the group homeworks as a vehicle for cooperative teaching and learning as well as a time-saving device. However, I do not want to see ‘carbon copies’ of the homework.

Regarding the group homeworks—some students fall into a trap of letting other members of their group do the hard intellectual work and think that they can catch up in time to take the exams. Of course, this is not only a mistake and not an effective way to learn—it is also bad manners.

You will be allowed one and only one late homework. No exceptions.

Final Grade: The grade will be determined by:

Homework (16%)

Homework is due in class on the assigned day with no exceptions except your one free late homework. The purpose of homework is to test your problem solving ability and help you prepare for exams.

Exam: 3 hourly exams and a final (84%)

Each hourly exam is worth 18% (every 3-4 weeks) and the final (cumulative) is worth 30%. Some exams may be take home. Please do not become complacent that you can find solutions to the questions without actually having to learn the material. Take home exams tend to be longer and more difficult than in class exams. Please try to keep up and work at a constant rate. Last minute studying for an exam is usually a recipe for poor performance.

Time Management: This is a 3 credit course. You are expected to spend 3 waking hours a week in lecture. You should be spending a minimum of eight hours a week reviewing lecture material, reading text book(s), doing homework, and studying for exams. My advice to you is that you spend at least 3 of those 8 hours reviewing lecture material each week—and that you set aside regular time to study.

Everything that will appear on the exams or the homeworks will be covered in the lectures, lecture notes and reading assignments. You will want to supplement the lecture notes with reading from the text or other sources on group theory.
**Outside Reading:** You should be doing a couple hours a week of reading. You are all mature enough to find readings on your own that supplement parts of the lecture that are hard to understand. *If you are having trouble finding outside reading for a particular - ask!*

**Additional Reference Material:** Any additional material will be placed in the Chem 509 folder on diamond3.

**Electronic Devices:** Students may use computers, laptops, and electronic tablets to follow/collect lecture notes. The use of these and other electronic (cell phones, iPods, etc.) for other purposes is not permitted during class.

**Academic Integrity:** Washington State University is committed to a learning environment that embraces academic honesty. In order to protect members of our community from results of dishonest conduct, the University has adopted policies to deal with cases of academic dishonesty. Please read, understand, and follow the academic policies on Academic Dishonesty found in the Standards for Student Conduct WAC 504-26-010 (3). The standards of Conduct for Students can be found at [http://conduct.wsu.edu](http://conduct.wsu.edu).

**Change in the rules for withdrawals:** There are no longer uncontested withdrawals so students cannot drop classes on the last day of instruction unless they cancel their entire enrollment. Students still have a total of four withdrawals during their career. The regular withdrawal deadline has been extended from week 9 to week 13. A student can use any of their withdrawals up until the end of week 13.

**Students with Disabilities:** Reasonable accommodations are available for students with a documented disability. Please notify the me during the first week of class of any accommodations needed for the course. Late notification may cause the requested accommodations to be unavailable. If you have a disability and may need accommodations to fully participate in this class, please visit the Disability Resource Center (DRC). All accommodations MUST be approved through the DRC (Admin Annex Bldg, Room 205). Please stop by or call 335-3417 to make an appointment with a disability specialist. Call 335-3417 or visit [http://accesscenter.wsu.edu](http://accesscenter.wsu.edu), Access.Center@wsu.edu if you have questions.

**Safety on Campus:** WSU has developed resources for the safety of students, faculty, staff and visitors. These are the Campus Safety Plan at [http://safetyplan.wsu.edu](http://safetyplan.wsu.edu) and the university emergency management at [http://oem.wsu.edu/](http://oem.wsu.edu/). You should also become familiar with the WSU ALERT site at [http://alert.wsu.edu](http://alert.wsu.edu) for information about emergencies affecting WSU. It is recommended that you go to the zzusis portal at [http://zzusis.wsu.edu](http://zzusis.wsu.edu) and register your emergency contact information for the Crisis Communication System (CCS).