Chemistry 507—F22

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Classroom Sessions: M, W, F 10:00 – 10:50 a.m., 1650 CHEM
Instructor Office Hours: TBD

Credits: 3

Course Content: Chem 507 demonstrates the interrelations of ideas presented in the fundamental inorganic chemistry curriculum. We will explore the role that electronic structure plays in governing the properties and reactivity of transition metal complexes. Starting from a foundational understanding of molecular symmetry and group theory, the course will build to cover contemporary topics in organometallic, bioinorganic, and energy science, as time allows. A more detailed outline of course content is provided below.

Required Texts:
Inorganic Chemistry Catherine Housecroft and Alan Sharpe, 5th Ed., Pearson
ISBN-13: 978-1292134147
Note: Other editions of this textbook are equally viable as it is largely used as a student resource and problems will not be assigned from the text.
Symmetry & Spectroscopy: an Introduction to Vibrational & Electronic Spectroscopy Daniel C. Harris & Michael D. Bertolucci, Dover
ISBN-13: 978-0486661445

Grading: Final grades will be determined by a combination of class participation, problem sets, and exams as follows:
Class Participation (20%)
Problem Sets (20%)
Primary Literature Assignments (10%)
Exam 1 (25%)
Exam 2 (25%)
Note: Grades will be posted on Canvas as they become available. They will be weighted appropriately; however, Chem 507 will be graded on a curve and this will not be reflected in the posted grades.

Note: The instructor **will only** consider reviewing *significant* grading errors on examinations within one week of students getting them back. Students must not alter their work in any way. Students should submit no more than one separate page by e-mail stating the grading errors clearly and concisely to the instructor. This statement must show that: 1) the answer key is incorrect or incomplete; 2) the answer provided is an equally valid solution; or 3) the answer provided matches that given in the key, but was not recognized as such. Correct answers buried within superfluous information and/or outright incorrect reasoning may be graded as wholly incorrect. Any changes in scoring will only occur through this formal process to assure grading integrity.

Note: Extra credit assignments will be made available at the instructor's discretion.

Class participation is comprised of multiple components designed to encourage student immersion in the course and provide professional development opportunities to hone skillsets that will be valuable throughout one's career as a scientist. To motivate critical evaluation of the primary literature, both contemporary and classic papers—relevant to the material being covered in class—will be posted on Perusall throughout the term. The use of Perusall (an available add-on in the course Canvas site) will encourage discourse by providing a platform for both individual and group annotations of chemistry article pdfs. In some instances, this might involve posting comments or responding to questions raised by the professor. In other cases, it will serve as a basis for open (but virtual) class discussion on a given work. Additionally, the Perusall platform can facilitate feedback, from both fellow students and the instructor. A second component of the participation grade aims to improve critical scientific thinking. At the end of the semester, students will be required to select a recently published scientific article and write a brief "peer review," mimicking

the process journal editors use prior to final publication. This process will be conducted iteratively with comments from both the student and the instructor.

Students are expected to complete problem sets throughout the term. **Collaborative work is encouraged** but each student must submit an individual assignment for grading. Assignments will be posted on Canvas and will be turned in prior to the start of lecture one week after they are released; answer keys will be posted two days after assignments are due. Late work turned in prior to the release of the answer key will be graded for a maximum of 50% credit. The problem sets will be graded, for completeness, on a scale of 1 to 5 with no partial credit. A grade of 5 represents a complete or near complete submission with entirely or almost entirely correct answers. A grade of 1 indicates serious gaps in knowledge demonstrated by incorrect answers and/or missing work. This grading scheme is clearly subjective; however, each assignment will be graded uniformly for every student in the course. Students are strongly encouraged to review the published answer keys even when scoring 4/5 on the homework sets to ensure complete understanding in preparation for the exams.

Chem 507 will have two take-home exams. Both will be cumulative—any material covered up to that point is fair game! The grading rubric for the exams will be clearly delineated, allowing students to make prudent decisions on the best use of available time. Exams must be completed individually, within the constraints provided. The midterm exam will be closed book and closed to class notes, with no resources permitted outside of those provided; the final exam will be open book and open to class notes. No collaboration is allowed on exams and no discussion of the exams with classmates is permitted until after the due date. Breaking these rules and cheating in any way is detrimental to your learning experience and disrespectful to your peers. It will not be tolerated (additional details below).

> ***Note:*** Students who have conflicts due to religious holidays, travel for U-M athletics, travel for your professional development, or health reasons may e-mail the instructor at least one week in advance to be excused from attending class and to make alternate arrangements for assignments due during your time away from class.
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> ***Note:*** Departmental policy indicates the first step in inquiring about the accuracy of a final grade should be directed to the lead instructor of the course. This initial inquiry should take place within the first fifteen University business days of the first full term following the term in which the disputed grade was issued. If, after this inquiry, the student is not satisfied with the instructor's response, the student may choose to initiate a formal grade grievance. To initiate a formal grade grievance, the student should contact the Associate Chair of Undergraduate Studies (ACUS) of the home department of the course in question before the end of the fifth week of classes in the first full term following the term in which the disputed grade was issued.

The problem sets and exams in Chem 507 are challenging, by design. As a graduate researcher in chemistry, you will be faced with questions that require deep analytical thinking and innovative problem solving. As a student in Chem 507, you will simulate these scenarios through the homework and exam questions—many of these are based off of topical literature content! Be mindful that pushing yourself aids in your development and, while challenging, the material and assessments in the course are doable with hard work, dedication to the class, and taking advantage of the resources available. This includes office hours, which are strongly encouraged. Often, a small hint or nudge in the right direction will save hours of frustration. The scheduling of both the exams is accomplished with student feedback and you should be prepared to dedicate at a *minimum* 15 hours of focused time for preparation for/execution of the exams. No problem sets or Perusall papers will be assigned the week prior to an exam to facilitate test preparation.

This semester, we will be implementing Avogadro–a freeware cross-platform molecular editing software–in Chemistry 507. A critical skill to success in Chemistry 507 is developing the ability to think about molecules in 3-D. Avogadro takes as input .txt files and will facilitate building molecules and visualizing both molecular structures and orbitals in three dimensions. The first week of class, a problem set will be posted to help you gain familiarity with this software. Work through this problem set as soon as possible so that we can catch and troubleshoot any problems early.

Each student in Chem 507 has had a different academic journey *en route* to this course. This is both a challenge and privilege with respect to course preparation and presentation. **I am confident that every student can be successful in this class with sufficient dedication and effort.** Content on assessments is covered in class and reinforced with recommended reading. If you ever feel that there is a topic that is not making sense, please reach out to the instructor.

Academic Integrity: There is a clear expectation that students will perform with honor and integrity. Students are referred to the LSA policy on academic integrity available online at:
https://lsa.umich.edu/lsa/academics/academic-integrity.html
Any student found by the Assistant Dean's office to have engaged in academic misconduct on exams will automatically fail the course.

Accessibility and Accommodations:
If you need an accommodation for a disability, please let me know at your earliest convenience. Some aspects of this course, such as the assignments, in-class activities, or the way we teach may be modified to facilitate your participation and progress. As soon as you make me aware of your needs, I can work with you, the Office of Services for Students with Disabilities, or the Adaptive Technologies Computing Site to help determine appropriate accommodations. I will treat any personal information with the utmost discretion.

Student Health and Well-Being:
LSA is committed to delivering our mission while aiming to protect the health and safety of the community, which includes minimizing the spread of COVID-19. As of May 2, 2022, the University of Michigan made mask use optional for indoor spaces (University's Face Covering Policy for COVID-19). The choice to wear (or not wear) a mask is a personal one and I encourage each of you to proceed in whatever way makes you the most comfortable. Note that this is subject to change over the course of the semester and each of us will be required to adjust appropriately.

For additional information on public health guidance, refer to the LSA Student Commitment to the Wolverine Culture of Care and the OSCR Addendum to the Statement of Student Rights and Responsibilities on the OSCR website.

The University of Michigan is committed to advancing the mental health and wellbeing of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of support, services are available. If you feel comfortable doing so, the first course of action should always be to speak with me. Open lines of communication are key to diagnosing and addressing problems. I will treat any personal information with the utmost discretion.

For a listing of other mental health resources available on and off campus, visit http://umich.edu/~mhealth/

Course Recording: The weekly lectures for Chem 507 will be held in person and simultaneously recorded for asynchronous posting online. As part of your participation in this course, you may be recorded. If you do not wish to be recorded, please contact the instructor during the first week of class (or as soon as you enroll in the course, whichever is latest) to discuss possible alternatives.

Class Conduct: A positive learning environment relies upon creating an atmosphere where diverse perspectives can be expressed and questions can be asked openly, without fear of negative repercussions. Each of us comes from a unique background and it is every member of the class's job to be understanding and respectful of differences in thought, prior training, viewpoint, and opinion. Respectful dialogue, be it in person or virtual, is expected and hostile or disrespectful behavior will not be permitted. Treat your peers as you would wish to be treated to establish a collaborative and supportive space for the exchange of ideas.

Requisite Background Knowledge: The list below constitutes prerequisite knowledge that will not be covered comprehensively in class. If you need to review, these topics are covered in the textbook.

- Electron configurations for atoms and ions
- Atomic orbitals: shapes & probability distribution functions
- Concept of effective nuclear charge & periodic trends (IE, EA, radii, electronegativity)
- Drawing 3-D representations of any molecule
- Balancing any chemical reaction (mass & charge)
- Using basic equations of thermodynamics & kinetics

You will find that these topics, and many other from your prior chemistry courses, will provide a foundation for the content in Chem 507. Connecting these concepts is critical to mastery of the material and success in this course.

Course Outline

I. Review of atoms & molecules, periodic properties, bonding in main group compounds, Lewis representations, and the VSEPR model. (**H&S Ch. 1 & Ch. 2**)

II. Symmetry
- A. Symmetry operations (**H&S 3.1-3.3 and H&B Ch. 1.1-1.3**)
- B. Point groups (**H&S 3.4 and H&B Ch. 1.4-1.5**)
- C. Matrix representations of symmetry operations (**H&B Ch. 1.6**)
- D. Character tables (**H&S 3.5-3.8 and H&B 1.7-1.8**)

III. Applications of group theory to LCAO/MO descriptions of polyatomics molecules (**H&S Ch. 5 and H&B Ch. 4.1-4.6**)

IV. Coordination chemistry of the transition metals
- A. Lewis acid – base theory (**H&S 7.7-7.13**)
- B. Dative bonding: σ donors, π donors, π acceptors (**H&S Ch. 20.4**)
- C. Ligand Field Theory (**H&S Ch. 20.4-20.5 & Ch. 20.11-20.13**)
- D. Classical complexes (**H&S Ch. 19 & Ch. 20**)
- E. π-Bonding in coordination compounds (**H&S Ch. 20.4, 24.2, & 24.5**)

V. Introduction to electronic spectroscopy of coordination compounds of high symmetry
- A. Electronic states and term symbols for free ions and metal complexes (**H&S 20.6 and H&B 5.3**)
- B. Selection rules (**H&S Ch. 20.7 and H&B Ch. 5.4**)
- C. Correlation diagrams (**H&S Ch. 20.7 and H&B Ch. 5.9**)
- D. Charge transfer spectra (**H&S Ch. 19.5 & Ch. 20.7 and H&B Ch. 5.9**)

VI. Strong field ligand systems
- A. Electron counting (**H&S Ch. 24.3**)
- B. The 18 electron "rule" (**H&S Ch. 24.3**)
- C. Formal oxidation states (**H&S Ch. 19.5-19.6**)

VII. Metal-ligand bonding, structure, and reactivity of important functional groups in transition metal compounds
- A. Carbonyl, isocyanide, nitrosyl, and dinitrogen complexes (**H&S Ch. 24.1-24.2**)
- B. Phosphine compounds (**H&S Ch. 24.1-24.2**)
- C. Cyclopentadiene compounds (**H&S Ch. 24.14-24.15**)
- D. Transition metal hydrides (**H&S Ch. 24.2**)
- E. Organometallic reactions [survey of elementary steps] (**H&S Ch. 24.8**)

VIII. Catalysis: Organometallics
- A. Reaction mechanism and kinetics (**H&S Ch. 25 & Ch. 26**)

VIV. Catalysis: Bioinorganic chemistry
- A. Balancing catalysis in metalloenzymes (**H&S Ch. 29**)

X. Special Topics (as time permits)