

Course Syllabus for Fall 2024  
Ch112 - Inorganic Chemistry (Tue/Thur, 1 PM, RSC 210)  
CCE, California Institute of Technology

**Instructor:**

Prof. Theodor Agapie  
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**Teaching Assistants:**

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**Office Hours** (147 Noyes)

TAs: Mondays 6 – 7 PM (Adjeoda) & Wednesdays 6 – 7 PM (Max)

Instructors: (Friday 11 AM – 12 PM), and by appointment

**Course Description:**

This course is designed to build upon introductory inorganic chemistry courses to give students the ability to describe electronic structures of more complicated inorganic complexes and use these descriptions to predict reactivity and spectroscopic properties. Experience is assumed with molecular symmetry, assignment of oxidation states, and electron counting.

**Course Welcome:**

We are excited to teach this graduate level course in inorganic chemistry! As a course typically taken by the incoming graduate students and advanced undergraduate, Ch 112 is designed to help students become proficient in employing fundamental concepts of group theory applied to bonding in order to analyze compounds of interest they may encounter in their research. Through examples from modern inorganic and organometallic chemistry, Ch 112 will teach students how to derive the electronic structure of simple as well as complex compounds. Based on the derived electronic structure, arguments about reactivity and spectroscopic properties will be developed. This course deals with a variety of molecules relevant to areas such as catalysis and small molecule activation which will provide students with experience with bonding motifs that they may encounter in their future chemistry endeavors. Lectures will primarily consist of synchronous on-line learning with virtual lectures and "in-class" exercises to allow students to practice in teams with instructor/TA guidance.

**Course Format:**

This course will be taught as a flipped classroom. Students are asked to watch recorded lectures before class time. When watching the lectures students are encouraged to submit any questions they have on Canvas under the "Discussions" section. Theo and TAs will try to address as many questions as possible at the start of class (or before), if submitted 24 hours in advance. Students will then work on problems during class time. The first part of the class period will focus on working through examples directly derived from the lecture; upon completing these, more challenging problems will be provided. Watching and understanding the lecture material before

class is essential to facilitate in class learning through problem solving. These problems will not count towards the students' grade.

### **Learning Outcomes:**

Upon successful completion of this course, you will be able to use molecular symmetry to derive molecular orbital diagrams of transition metal complexes. You will be able to use them to predict reactivity with small molecules and to predict spectral features.

- Determine molecular symmetry, utilize matrix representations, and use character tables to derive molecular orbital diagrams.
- Utilize molecular orbital diagrams, projection operators, and knowledge of molecular orbital interactions to predict:
  - The interaction of  $\pi$  systems with transition metals.
  - The interaction/activation of small molecules ( $N_2$ , CO,  $O_2$ ,  $CO_2$ ) with transition metal complexes.
  - The interaction of transition metals with individual elements (nitrides, carbides, oxos) and with other metals (metal-metal bonding).
  - The electronic states of complexes and their possible excited states.
- Utilize molecular orbital diagrams and character tables to predict/explain electronic absorption spectroscopic properties.
- Understand how electronic structure can be used to predict complexes' chemical reactivities.

### **Textbooks:** (recommended, not required)

Lectures will cover all material you are responsible for on exams.

Symmetry and Spectroscopy, Harris and Bertolucci. (Highly recommended, not required)

Inorganic Chemistry, Miessler, Fischer and Tarr. (Useful as another reference, not required)

### **Course Website or Learning Management System:**

All course material will be available on Canvas.

Canvas will be used for course messages, assignments, lecture zoom recordings, course material, and posting grades.

GradeScope will be used for uploading completed problem sets and exams. Please submit your problem sets as a single pdf (using a free scanning app, e.g., CamScanner or Adobe Scan), with each problem started on a separate page.

### **Grading Overview:**

#### **Problem sets (6): 16% of total grade**

Weekly problem sets will be available online on Friday and will be due on the following Thursday, at the start of class. Each problem set will be graded on a 0-10 scale, in whole point increments. Graded problem sets will not be corrected in detail. You are encouraged to cross-check your worked problems with the solutions that are made available.

**Project: 12%**

Written summary on a current topic in inorganic chemistry (~60%) and a section (~40%) on a new direction / proposal of original research if you were to work in the area of the project (4 pages not including references, JACS format). It is expected that the project will be designed to emphasize aspects learned in class. It is helpful to think about drafting the paper (and your oral presentation) as a tool to teach your classmates, TAs, and instructors about the topic and proposal of your choice. You are encouraged to make use of Gaussian/ in your project. Due on Nov 21. Abstract (1%) due on Oct 17. Topic selection (three choices) due on Oct 10.

**Paper critique: 4%**

Each student will select a paper from recent literature (from JACS, Angewandte, Science, Nature) focused on an aspect related to your selected project topic. See below on format of critique. Due on Oct 17.

Brief summary of major findings and conclusions

Significance: importance of questions being addressed

Approach: are the methods appropriate to answer the questions?

Innovation

Data: quality and reliability

Conclusions: do the data adequately support the conclusions; are there reasonable alternative interpretations?

Do the results challenge existing interpretations or support accepted concepts?

Do the results develop new concepts, point to new research directions or to new paradigms?

Turn in 0.5-1 page written critique (12 pt Arial, single space)

**Presentation: 8% (including class participation)**

Lecture time in the last week will be reserved for student oral presentations of the projects. Time limit for presentation is 9 minutes; practice being concise! Prepare no more than 6 slides (4 on background, 2 on the proposed new direction). Students in the audience are expected to participate with questions and comments. Turn in the slides to the TAs as a pdf file by 10 pm the day before the presentation. More information and rubric will be posted on Canvas closer to presentation date.

**Exams:**

**Midterm (30%), final (30%).** Closed book, take-home. Consultation of test materials from previous years is not allowed.

**Attendance and Participation:**

Attending lecture and participating in in-class exercises will be essential to success on problem sets and exams as well as in learning the material for use in future endeavors. All exam material is based on lecture material. In-class exercises and problem sets will provide students with ample practice opportunities for exam questions.

### **Academic Integrity:**

Caltech's Honor Code: "No member of the Caltech community shall take unfair advantage of any other member of the Caltech community."

### **Understanding and Avoiding Plagiarism:**

Plagiarism is the appropriation of another person's ideas, processes, results, or words without giving appropriate credit, and it violates the honor code in a fundamental way. You can find more information at: <http://writing.caltech.edu/resources/plagiarism>.

### **Collaboration Policy:**

Students are encouraged to collaborate and discuss problem sets with each other. However, the final problem set that is turned in must be the student's original work. Consultation of test materials from previous years is not allowed.

To facilitate collaboration on learning course material, students are encouraged to post questions to Canvas in the "Discussions" section. Other students are encouraged to answer these questions and TA's and professors will also monitor these discussions and provide answers/comments as necessary.

### **Students with Documented Disabilities:**

Students who may need an academic accommodation based on the impact of a disability must initiate the request with Caltech Accessibility Services for Students (CASS). Professional staff will evaluate the request with required documentation, recommend reasonable accommodations, and prepare an Accommodation Letter for faculty dated in the current quarter in which the request is being made. Students should contact CASS as soon as possible, since timely notice is needed to coordinate accommodations. <http://cass.caltech.edu/>.

Undergraduate students should contact Dr. Lesley Nye, Associate Dean of Undergraduate Students (administrative contact: Beth Larranaga) and graduate students should contact Dr. Natalie Gilmore, Associate Dean of Graduate Studies (administrative contact: Georgine Okura).

### **Due Dates**

PS1 + Topic Choice	Oct 10
Critique/Abstract	Oct 17
PS2	Oct 24
PS3	Oct 31
Midterm	Nov 7
PS4	Nov 14
PS5	Nov 21
Report	Nov 26
PS6	Dec 5
Presentations	Dec 3 and Dec 5
Final	Dec 12