

Chem236: Physical Inorganic Chemistry, 3.0 credits

Spring 2022 Lecture

TR 8:30 – 9:45 AM, Lafayette L102

Instructor

Prof. Matt Liptak

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Office Hours

W 11 AM-12 PM, F 10-11 AM, Innovation E336

Prerequisites

Chem131 and Chem165 OR Chem231

General Education Requirements

This course does **not** satisfy any general education requirements

Chem236 does partially satisfy the *College of Arts and Sciences Natural Sciences* distribution requirement.

Chem236 is an acceptable *advanced elective* for the **Chemistry majors**.

Chem236 is an acceptable *advanced elective* for the **Biochemistry major**.

Course Description

Determination of molecular and electronic structure of inorganic complexes using spectroscopic techniques. Introduction to magnetism. Interpretation of spectroscopic data within the frameworks of group theory and electronic structure calculations.

Course Learning Objectives

Upon completion of Chem 236, it is anticipated that you will:

1. Identify appropriate physical characterization tool(s) for an inorganic species of interest.
2. Describe the sample and instrumentation requirements for these techniques.
3. Analyze spectroscopic data using group theory and electronic structure calculations.
4. Understand physical characterizations of inorganic species described in the literature.

Textbook

Required: Que, Lawrence Jr. *Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism*, University Science Books, 2000.

Recommended: Cramer, C.J. *Essentials of Computational Chemistry*, Wiley, 2004.

Miessler, G.L.; Fischer, P.J.; Tarr, D.A. *Inorganic Chemistry*, Pearson, 2014.

Web Content

Lecture notes, problem sets, problem set answer keys, and exams will be available through Blackboard (bb.uvm.edu). These materials are available for all current, UVM-affiliated, students, but they may not be shared off-campus without permission of the instructor.

The instructor reserves the right to change everything, with notice

Attendance Policy

I do not take attendance in Chem236, but you are expected to attend all lectures. If you miss lecture for any reason, it is **your** responsibility to catch-up on missed material by reviewing the materials posted to Blackboard.

Grading –Graduate students

Exams (50%): Two exams are scheduled for Chem 236. These exams are *not* cumulative. The first exam will be on **Thursday, March 3 at 8:30 AM**. The second exam will be on **Tuesday, May 10 at 7:30 AM**.

Problem Sets (25%): A total of 6 open-book, open-notes problem sets will be assigned throughout the semester. Problem sets are due at **10:05 AM** on the due date. Late Problem sets will not be accepted, but the lowest score will be dropped.

Class Presentation (25%): Each student will give a 30 minute presentation on an experimental or theoretical characterization method not already covered by this course. Popular topics from past years include Luminescence spectroscopy, Mössbauer spectroscopy, and X-ray crystallography.

Grading – Undergraduate students

Exams (67%): Two exams are scheduled for Chem 236. These exams are *not* cumulative. The first exam will be on **Thursday, March 3 at 8:30 AM**. The second exam will be on **Tuesday, May 10 at 7:30 AM**.

Problem Sets (33%): A total of 6 open-book, open-notes problem sets will be assigned throughout the semester. Problem sets are due at **10:05 AM** on the due date. Late Problem sets will not be accepted, but the lowest score will be dropped.

Statement on Diversity and Inclusion

I strive to create a classroom environment that supports students from a diverse set of backgrounds. Our society is composed of individual from diverse ethnic, socioeconomic, and educational backgrounds. Half of our society are women. I strongly believe that our best path forward to a stronger and more equitable society is to promote inclusiveness.

It is my expectation that every member of this class will also support diversity and inclusion. As a community, we should strive to uphold the ideals of Our Common Ground:

<https://www.uvm.edu/president/our-common-ground>

I welcome any suggestions as to how I can promote a diverse and inclusive classroom.

Course Evaluations

All students are expected to complete course evaluations on **May 5**. The evaluations will be anonymous and confidential. The information gained from these evaluations will be used to iteratively improve Chem236 for future *UVM* students.

General statement regarding potential changes during the semester:

<http://catalogue.uvm.edu/>

The University of Vermont reserves the right to make changes in the course offerings, mode of

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delivery, degree requirements, charges, regulations, and procedures contained herein as educational, financial, and health, safety, and welfare considerations require, or as necessary to be compliant with governmental, accreditation, or public health directives.

Green and Gold Promise:

The [Green and Gold Promise](#) clearly articulates the expectations that UVM has for students, faculty, and staff to remain compliant with all COVID-19 recommendations from the federal CDC, the State of Vermont, and the City of Burlington.

The [Code of Student Conduct](#) outlines policies related to violations of the Green and Gold Promise. Sanctions for violations include fines, educational sanctions, parent notification, probation, and suspension.

Intellectual Property Statement/Prohibition on Sharing Academic Materials:

Students are prohibited from publicly sharing or selling academic materials that they did not author (for example: class syllabus, outlines or class presentations authored by the professor, practice questions, text from the textbook or other copyrighted class materials, etc.); and students are prohibited from sharing assessments (for example homework or a take-home examination). Violations will be handled under UVM's Intellectual Property policy and Code of Academic Integrity.

Student Learning Accommodations

In keeping with University policy, any student with a documented disability interested in utilizing accommodations should contact SAS, the office of Disability Services on campus. SAS works with students and faculty in an interactive process to explore reasonable and appropriate accommodations, which are communicated to faculty in an accommodation letter. All students are strongly encouraged to meet with their faculty to discuss the accommodations they plan to use in each course. A student's accommodation letter lists those accommodations that will not be implemented until the student meets with their faculty to create a plan.

Contact SAS:

A170 Living/Learning Center;
802-656-7753;
access@uvm.edu
www.uvm.edu/access

Religious Holidays

Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of your absence to me in writing by the end of the second full week of classes. You will be permitted to make up work within a mutually agreed-upon time. <https://www.uvm.edu/registrar/religious-holidays>

Academic Integrity

The policy addresses plagiarism, fabrication, collusion, and cheating.
<https://www.uvm.edu/policies/student/acadintegrity.pdf>

Grade Appeals

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If you would like to contest a grade, please follow the procedures outlined in this policy:

<https://www.uvm.edu/policies/student/gradeappeals.pdf>

Grading

For information on grading and GPA calculation, go to <https://www.uvm.edu/registrar/grades>

Code of Student Conduct

<http://www.uvm.edu/policies/student/studentcode.pdf>

FERPA Rights Disclosure

The purpose of this policy is to communicate the rights of students regarding access to, and privacy of their student educational records as provided for in the Family Educational Rights and Privacy Act (FERPA) of 1974.

<http://catalogue.uvm.edu/undergraduate/academicinfo/ferparightsdisclosure/>

Promoting Health & Safety

The University of Vermont's number one priority is to support a healthy and safe community:

Center for Health and Wellbeing

<https://www.uvm.edu/health>

Counseling & Psychiatry Services (CAPS)

Phone: (802) 656-3340

C.A.R.E.

If you are concerned about a UVM community member or are concerned about a specific event, we encourage you to contact the Dean of Students Office (802-656-3380). If you would like to remain anonymous, you can report your concerns online by visiting the Dean of Students website at <https://www.uvm.edu/studentaffairs>

Final Exam Policy

The University final exam policy outlines expectations during final exams and explains timing and process of examination period. <https://www.uvm.edu/registrar/final-exams>

Statement on Alcohol and Cannabis in the Academic Environment

As a faculty member, I want you to get the most you can out of this course. You play a crucial role in your education and in your readiness to learn and fully engage with the course material. It is important to note that alcohol and cannabis have no place in an academic environment. They can seriously impair your ability to learn and retain information not only in the moment you may be using, but up to 48 hours or more afterwards. In addition, alcohol and cannabis can:

Cause issues with attention, memory and concentration

Negatively impact the quality of how information is processed and ultimately stored

Affect sleep patterns, which interferes with long-term memory formation

It is my expectation that you will do everything you can to optimize your learning and to fully participate in this course.

Tentative Lecture Schedule		
Monday	Tuesday	Thursday
Jan. 17	Molecular Orbitals (MF&T 5.4,10.3-10.4)	Electronic States (MF&T 10.3-10.5,11.2)
Jan. 24	Density Functional Theory (Cramer 8.1-8.3)	Exchange-Correlation Functionals (Cramer 8.4)
Jan. 31	Electronic Absorption (Que 1.1-1.8) PS #1 Due	Charge Transfer (Que 1.9-1.11)
Feb. 7	Ligand Field (Que 1.12-1.17)	TDDFT (Cramer 14.1-14.3)
Feb. 14	IR and Raman (Que 2.1-2.2) PS #2 Due	Molecular Vibrations (Que 2.3)
Feb. 21	Resonance Enhancement (Que 2.4)	Frequency Calculations (Cramer 9.3)
Feb. 28	Town Meeting Day PS #3 Due	Exam #1
Mar. 7	Spring Recess	Spring Recess
Mar. 14	Spin-orbit Coupling (Que 3.1-3.2A)	Spin-Spin Coupling (Que 3.2B-3.2F)
Mar. 21	Hyperfine Coupling (Que 3.3)	CP-SCF (Cramer 9.1)
Mar. 28	CD Spectroscopy (Que 5.1-5.7) PS #4 Due	MCD Spectroscopy (Que 5.8-5.9A)
Apr. 4	VTVH MCD (Que 5.9B-5.11)	CAS-SCF (Cramer 7.1-7.4)
Apr. 11	Hyperfine Shift (Que 8.1A-8.1B) PS #5 Due	Paramagnetic Relaxation (Que 8.1C-8.1D)
Apr. 18	Two-dimensional NMR (Que 8.2)	NMR Resonance Assignment
Apr. 25	Graduate Student Presentation Day PS #6 Due	Graduate Student Presentation Day
May 2	Graduate Student Presentation Day	Graduate Student Presentation Day

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