CHEM 4715/8715: PHYSICAL METHODS IN INORGANIC CHEMISTRY Fall 2023; 3 credits

Syllabus

Instructor	Dr. Gwen Bailey	
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Pronouns: she/her/hers

Class MWF, 12:20 – 1:10 PM, Smith 111

Office Hours TBD

Website Canvas

Welcome to CHM4715/8715! Inorganic chemistry as a discipline is founded upon a detailed understanding of the electronic structure, bonding and mechanism in its constituent compounds. Detailed physical interrogation is required to advance the field and understand new compounds and reaction chemistry.

In this course, you will gain an understanding and appreciation for the common physical characterization techniques used to probe atom connectivity, electronic structure, and bonding in inorganic compounds. While our focus will be on molecularly precise, homogeneous compounds, many of the methods we will study can equally be employed to heterogeneous systems. You will have the opportunity to explore modern concepts in inorganic research, including how physical characterization techniques support and advance seminal topics in the field. You will also be invited to tailor many of the activities, such as writing assignments, essays, etc., to your research interests.

<u>Topics</u>: NMR and EPR spectroscopy, electrochemistry, DFT, magnetism, Mössbauer spectroscopy, X-ray absorption spectroscopy, vibrational and electronic spectroscopy, mass spectrometry.

<u>Formal prerequisites</u>: CHEM 4701 or equivalent; chem major or instructor consent. Basic familiarity with fundamental concepts in inorganic chemistry is assumed.

Learning outcomes – by the end of this course, you will be able to:

1. Rationalize and explain the shapes and axes of common data; interpret and draw conclusions from datasets

2. Propose physical experiments to address questions about inorganic structure and reactivity

3. Critically evaluate and discuss the application of physical inorganic methods to modern problems

4. Extend the understanding and skillsets developed in class to more advanced and specialized physical characterization methods

Textbooks:

- **Required**: *Structural Methods in Molecular Inorganic Chemistry*, by Rankin, Mitzel, and Morrison 3 copies are on reserve at Walter library; otherwise \$60 (Amazon) or \$42 (e-book, VitalSource*)
- Optional: Physical Methods for Chemists, by R. S. Drago (electronic copy available upon request)

*This textbook is provided through the Inclusive Access program on the Canvas CHM4715/8715 website. Pricing for the e-book through this program is reduced, <u>but you must opt out of the program if you wish</u> to purchase or obtain your materials elsewhere. More details are provided below.

COURSE FORMAT

Reading assignments (10 pts)

Participation will be assessed via a short pre-class quiz. The quizzes will be assessed on a complete/incomplete basis for 10 pts. What is important is not that you understand everything prior to coming to class, but that you use the readings and quiz questions to engage with the material. Doing so will ensure that you come to class prepared to assimilate the course content and ask questions.

Participation (20 pts)

Participation will be judged in both small and large group activities throughout the course, since both are essential for learning in the course. Small group activities will use POGIL (Process-Oriented Guided Inquiry Learning), an evidence-based method shown to improve learning and equity in STEM fields. More information can be found here: <u>https://pogil.org/.</u> In addition, literature case studies will be completed collaboratively in groups and handed in for participation marks. Assessment will be based on both engagement and correctness.

Problem sets (20 pts)

Questions from the problem sets will ask you demonstrate your understanding and grapple with key concepts. Problem sets will be completed partly in class, and partly at home, and will be graded for correctness. Students are advised to write the answers to problem sets in class and not wait until they get home to transcribe the answers; use of pencils can help in case corrections need to be made.

<u>Collaboration policy</u>: While collaboration is allowed on problem sets, each collaborator is expected to contribute to all problems and turn in individual answers. The solution must be presented and explained in your own words and following your own logic for full points. Collaborators must be listed on each problem set.

Written assignments (20 pts)

Writing assignments will be your opportunity to engage and critically reflect on impactful pieces of modern literature in which physical characterization methods are discussed.

CHEM 8715: three written assignments worth 3, 7, and 10 pts

CHEM 4715: the third written assignment is optional

Student Lecture (15 pts)

Students will present a 15-minute lecture on a physical method of interest to them which has not been covered in class. Topics may be chosen from the provided list or approved by the instructor. As part of the assignments, graduate students will discuss application of the method to an impactful problem of modern interest. Student lecture dates will be on Friday, Oct 6, 13, and 20. You must sign up for a topic and date by Friday, Sept 15.

Final Exam (15 pts)

This will be a closed-door, closed-book 1:1 oral exam where students will be assessed on both breadth and depth of their knowledge. A practice final exam will be held in groups on the final day of instruction (Dec 8). The last week of instruction (Dec 11 & 13) will be cancelled and instead oral exams will be scheduled individually with the students. Possible questions include (but are not limited to):

- 1. Tell me about the theory behind [insert physical method]. What is it that we are measuring, and what can it tell us about the system we are studying?
- 2. Design a comprehensive characterization plan for [insert molecule] that will elucidate both the atomic configuration and electronic structure. Be as specific as you can about which methods you will apply and what you plan to learn from those methods.
- 3. Interpret and draw conclusions from [insert physical characterization data].

GRADING:	Reading assignments	10 pts
	Problem sets	20 pts
	In-class participation	20 pts
	Writing Assignments	20 pts
	Student Lecture	15 pts
	Final Exam	15 pts
	<u>Total</u> :	<u>100 pts</u>

<u>Calculation of grades</u>: A: 100-90%, A⁻: 89-85%, B⁺: 84-80%, B: 79-75%, B⁻: 74-70%, C⁺: 69-65%, C: 64-60%, C⁻: 59-5%, D: 54-50%, F: <50%. **Grading curves will not be applied.**

<u>COURSE SCHEDULE</u> – subject to change

Week of	Торіс	Reading	Friday	Due
Sept 6	NMR spectroscopy	Ch 4.2, 4.4, 4.18		
Sept 11			Sept 15	Written assignment 1 Lecture topics due
Sept 18	EPR spectroscopy	Ch 5.1-5.3, 5.5	Sept 22	Sept 22: PSet 1 (NMR)
Sept 25				
Oct 2			Oct 6	Student lectures
Oct 9	DFT	Ch 3.1-3.2, 3.7-3.9	Oct 13	PSet 2 (EPR) Student lectures
Oct 16			Oct 20	Student lectures
Oct 23	Electrochemistry		Oct 27	Written assignment 2
Oct 30		Ch 6.1-6.4		
Nov 6	Magnetism		Nov 10	PSet 3 (Electrochemistry)
Nov 13	Mossbauer	<i>J. Chem. Ed.</i> 2018 197 <i>NCR</i> 2017 0039		
Nov 20			Nov 24	PSet 4 (Magnetism)
Nov 27	X-ray absorption spec- troscopy	Ch 9.1-9.3 Ch 8.1-8.3, 8.8	Nov 17	Written assignment 3
Dec 4	Special topics Final exam practice			
Dec 11	Final exam		Dec 15	PSet 5 (Mössbauer)

CLASS POLICIES For a complete list, see: https://policy.umn.edu/education/syllabusrequirements-appa

COVID-19, Face-Coverings, Symptoms, and Vaccination

Stay at home if you experience any signs of illness or have a positive COVID-19 test result, and consult with your healthcare provider about an appropriate course of action. Absences related to illness, including COVID-19 symptoms, for yourself or your dependents, are <u>excused absences</u> and I will work with you to find the best course of action for missed work and course content. I will follow these same protocols and will let you know if the delivery of this course has to be temporarily changed as the result of my own circumstances.

In-class discussions: The learning activities in this course will center heavily around in-class problem solving and discussions. Students are invited to engage in these discussions as a part of the learning process, including taking risks, testing ideas, and encouraging one another. As your instructor, I will take steps to foster a learning environment where every student can thrive, regardless of their own individual identities. However, I am not omniscient and so I encourage you to voice concerns of any kind with me so that resolution can be sought. Alternatively, students may seek support from the student ombuds office (for more information, visit http://sos.umn.edu/ombuds).

Late assignments: A penalty of 50% will be applied for late assignments. An assignment will be considered late if it is not submitted by 11:59 PM on the assignment deadline. Accommodations will be applied for reasonable requests, if the instructor is contacted in advance of the deadline.

Textbook Inclusive Access: You have enrolled in a course using Inclusive Access (IA). This means your course materials will be delivered electronically to the Canvas course website. They will be available by the first day of class, and you will be charged automatically for them through your student account. You will access your IA course materials through the course page in Canvas.

Instructions for opting out of the program. If you do not want to participate in the IA program, you can opt out of the access and the fee will be refunded as long as you opt out before the deadline. The Bookstores will send an IA welcome email near the beginning of the semester, and this email will have instructions about how to opt out and when the deadline is for opting out. Typically you have about a week into the semester to opt out. The welcome email will also contain other useful information about IA, so please watch for it (sender: <u>no-reply@verbasoft-ware.com</u>). If you have any questions about IA, please contact the Bookstores at <u>inclusiveaccess@umn.edu</u>.

Accommodations: The University of Minnesota views disability as an important aspect of diversity, and is committed to providing equitable access to learning opportunities for all students. The Disability Resource Center (DRC) is the campus office that collaborates with students who have disabilities to provide and/or arrange reasonable accommodations. See https://diversity.umn.edu/disability/ or email drc@umn.edu.

- If you have, or think you have, a disability in any area such as, mental health, attention, learning, chronic health, sensory, or physical, please contact the DRC office on your campus (UM Twin Cities 612.626.1333) to arrange a confidential discussion regarding equitable access and reasonable accommodations.
- Students with short-term disabilities, such as a broken arm, can often work with instructors to minimize classroom barriers. In situations where additional assistance is needed, students should contact the DRC.
- If you are registered with the DRC and have a disability accommodation letter dated for this semester or this year, please contact your instructor early in the semester to review how the accommodations will be applied.

Mental health & stress management: As a student you may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. University of Minnesota services are available to assist you. You can learn more about the broad range of confidential mental health services available on campus via the Student Mental Health Website: http://www.mentalhealth.umn.edu.

Incomplete grade: A student may request an Incomplete only when (a) there is a University-sanctioned excuse for missing the final exam and (b) the student is passing the course based on all other graded components. Assignment of an I requires that the instructor and student sign a contract, available in the Departmental undergraduate office, stipulating the procedure by which the I grade will be made up (e.g., taking a final exam from another instructor in the next semester). Failure to successfully complete the procedure outlined in the contract will result in the I being administratively changed by the University Registrar to an F or N (depending on the grade base) one calendar year from the end of the semester for which the I grade was granted. Note that the University has policies already in place to permit students called to military service, or unexpectedly disabled by major medical issues, to petition for withdrawal (and potential full or partial tuition remission) without prejudice.

Scholastic dishonesty

The U of M Student Conduct Code defines scholastic dishonesty as: "plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis." A student responsible for scholastic dishonesty can be assigned a penalty up to and including an "F" or "N" for the course.

Grading disputes

To dispute a grade, you must submit a written request within 48 hours of receiving the grade. In the written request, you should state and justify specific reasons for why you think your answer is acceptable or a higher grade is deserved.

More information about UMN policies can be found here: https://policy.umn.edu/education/syllabusrequirements