UNIVERSITY OF TEXAS AT TYLER

FALL 2024

SYLLABUS

THURSDAY 6-8:45 PM
RBS 2015

CHEM 5339.001
Bioinorganic Chemistry

Dr. Jason Smee

Contact Info

- jsmee@uttyler.edu
- 903.566.7069
- RBS 3030

Office Hours

- MWF 10:30-11:30
- TR 9-10 am
- and by appointment

Inside the Syllabus

Other Resources	2
Student Learning Outcomes	2
Course Requirements	2
Canvas	2
In-Class Presentation	3
Homework	3
Midterm and Final Exams	3
Grading	4
Topics Covered	4
Tentative Schedule: Topics & HW	5
University Policies	6-7

Course Description

Study of the role metal ions play in the structure and function of nucleic acids, proteins, and metalloenzymes. Topics include bio-coordination chemistry, modeling studies, and experimental techniques, as well as aspects of medicinal inorganic chemistry (time permitting).

Bioinorganic (adjective): of, relating to, or concerned with the application of inorganic chemistry and its techniques (as nuclear magnetic resonance) to the study of biological processes and substances (as metalloproteins) in which inorganic substances are important constituents or play important roles

- Merriam-Webster dictionary

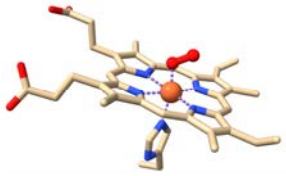
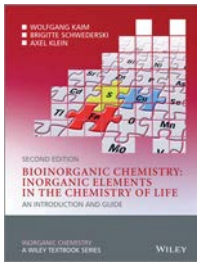


Image generated using *ChimeraX* software; data taken from structure 3A0G in the Protein Data Bank.

Recommended Materials



The recommended text is *Bioinorganic Chemistry -- Inorganic Elements in the Chemistry of Life: An Introduction and Guide*, 2/e by Kaim, et al. (ISBN 978-1-118-13807-6978-0-470-97523-7)

(Image from https://www.wiley.com.)

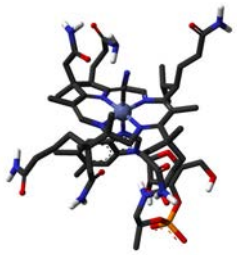
A scientific calculator (capable of exponents and logarithms) is **required**.

(Image from https://www.schoolspecialty.com/casio-scientific-calculator-035399.)

Important Dates

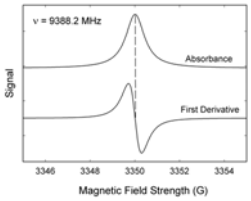
(Note: exam/presentation dates are tentative)

- September 9 (Friday): Census Date; last day to file for grade replacement
- October 1 (Tuesday): Last Day to File for Fall Graduation
- **October 17: Exam 1**
- November 4 (Monday): Last Day to Drop with a "W"
- November 11 (Monday): Last Day to Schedule Thesis Defense for Fall Graduation
- **November 21: Exam 2**
- November 25—29: Thanksgiving, no classes
- **December 5 (Thursday): Presentations , part 1**
- **December 12 (Thursday): Presentations, part 2**



Cobalamin, also known as vitamin B12 (shown here as the cyano complex), was the first known bioinorganic compound. It plays a significant role in many biological processes. (Image from Wikipedia.)

Crystal structure of human ferredoxin-1. Ferredoxins are one type of iron and sulfur-containing proteins that involved in a wide variety of electron transfer processes. (Image from Wikipedia)



Electron paramagnetic/spin resonance (EPR or ESR) is a form of spectroscopy similar to NMR, but instead of nuclei, it looks at unpaired electrons. Interestingly, EPR/ESR spectra are usually plotted as the first derivative. (Image from Wikipedia.)

Other Useful References

- Bioinorganic textbooks: *Inorganic Chemistry* 6/e by Shriver et al. 9781429299060; *Bioinorganic Chemistry: A Short Course*, 3/e by Roat-Malone 9781119535218; *Principles of Bioinorganic Chemistry* by Lippard and Berg 9780935702736; *Biological Inorganic Chemistry* by Bertini et al. 9781938787966
- Medicinal inorganic textbooks: *Metals in Medicine* by Dabrowiak (9780470681961); *Medicinal Inorganic Chemistry* by Sessler (978-0195686982)
- Chem LibreTexts website: the Bioinorganic book and the "Spectroscopy" supplementary module to Physical and Theoretical Chemistry
- UTT library website (library.uttyler.edu) for the following class-related activities:
  - classic and current bioinorganic/medicinal inorganic articles
  - a 15-minute oral presentation on a current article related to this course
- Need off-campus library access? Go to the Connecting from Off-Campus page.

Student Learning Outcomes

By the end of this course, students should be able to

1) Interpret results of characterization techniques used in bioinorganic studies
2) Recognize the different roles played by metalloproteins and metalloenzymes
3) Extract key concepts from classic and current journal articles
4) Effectively present, in seminar format, a summary of the results of a journal article relating to bioinorganic or medicinal inorganic chemistry

Course Requirements

1) One semester of undergraduate or graduate inorganic chemistry and one semester of undergraduate or graduate biochemistry are suggested.
2) We meet Thursdays from the weeks of Aug 29 to Dec 2, except during Thanksgiving (Nov 25—29). Attendance will be taken and class participation will be sought to nurture student communication and presentation skills.
3) You will be required to give a 15-minute presentation over a journal article obtained from such sources as *Inorganic Chemistry*, *Journal of Biological Inorganic Chemistry*, and *Journal of Inorganic Biochemistry*.
4) There are 2 midterm exams only (no comprehensive final exam).
5) In-class homework and traditional homework exercises will also be assigned.

Canvas

I will utilize Canvas to post such things as the syllabus, lecture notes, any Zoom recording links needed, assignments, and grades. The official gradebook is, however, the Excel spreadsheet on my desktop computer

canvas

In-Class Presentation

1) Near the end of the semester you will be asked to give a 10-15 minute presentation summarizing the results of a recent (within the last 5 years) article or communication (i.e. a mini-article) relating to bioinorganic or medicinal inorganic chemistry. If you are unsure of whether a paper is suitable, please ask me. Good journals to look through are *Journal of Biological Inorganic Chemistry* (SBIC), *Journal of Inorganic Biochemistry* (Elsevier), and *Inorganic Chemistry* (ACS); although there are others (e.g., *Biochemistry* by ACS).
2) Your paper must include one of the physical methods topics discussed in class.
3) ***The paper must be pre-approved by me. NO REVIEW ARTICLES!***
4) The grade will be based primarily on organization, style, clarity, and the ability to answer questions related to this course. A rubric will be provided to help with the planning of your presentation.
5) The presentation will be worth 20% of the course grade.
6) You will need to upload a copy of your presentation to Canvas when you are finished. A grade for the presentation will not be posted until the presentation has been uploaded.

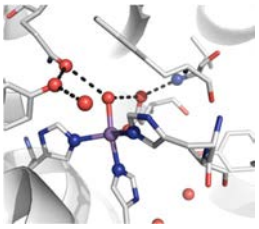
Homework

Homework (40% of the course grade) is comprised of

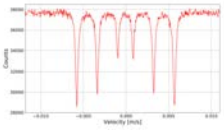
1) problem sets, both in-class groupwork and take-home; and
2) questions regarding assigned reading of classic and current papers. Assignments will be due at the beginning of the next class.

Midterm Exams

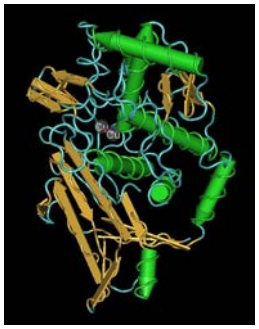
1) Two mid-term exams will be given during class time and are collectively worth 40% of your overall grade (20% each). They will be a mixture of short answer/ calculation questions and multiple choice. I will inform you where the material will be cutoff at least one week before the exam.
2) There is no final exam, comprehensive or otherwise.
3) Missed exams due to an unexcused absence will result in a grade of zero. In the event of an excusable situation, please give me at least two days' notice (if possible) to schedule an alternate time.
4) Cell phones, smart watches, and any similar electronic devices must be turned off and put away during exams. If they observed out in a visually accessible place (i.e. between legs, on the floor, etc.), it will be assumed that they are being used to cheat; your exam will taken away, you will receive a zero score (0 points) for the test, and you will be referred to the Office of Judicial Affairs.



Active site of human manganese superoxide dismutase (SOD). SOD converts superoxide O_2^- into O_2 and H_2O_2 and is one of several enzymes that deal with oxidative stress. (Image from Wikipedia.)



Mössbauer spectroscopy is a technique that relies upon the nearly recoil-less absorption of gamma rays and is very sensitive to the chemical environment of the sample. By far, the most commonly studied element is iron. (Image from Wikipedia.)

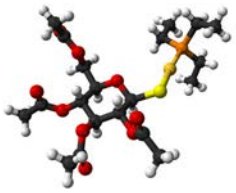


Crystal structure of octopus hemocyanin. Hemocyanin is a O_2 transport protein used by some invertebrates. The active site consists of two copper(I) ions that, upon binding O_2, are oxidized to copper(II) resulting the blue (cyan) color. (Image from Wikipedia.)

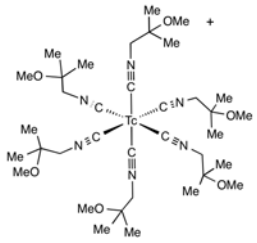
Grading

- All grades will be posted on Canvas.
- Course grades will be tentatively based on a 90/80/70 scale, but may be adjusted based on my evaluation of the class's overall performance.
- The official gradebook is the Excel spreadsheet on my office desktop.

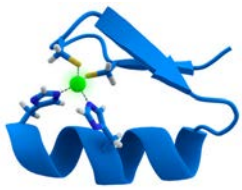
In-Class Presentation	20%
Homework	40%
2 Midterm exams	40%
Total	100%



Auranofin (Ridaura™) is a gold-phosphine thiolate complex that was a first-generation therapeutic used in the treatment of rheumatoid arthritis. (Image from Wikipedia.)



Technetium (^{99m}Tc) sestamibi (sesta = 6; MIBI = methoxyisobutylisonitrile). Known under the trade name Cardiolite™ this contrasting agent is primarily used to image heart muscle. (Image from Wikipedia.)

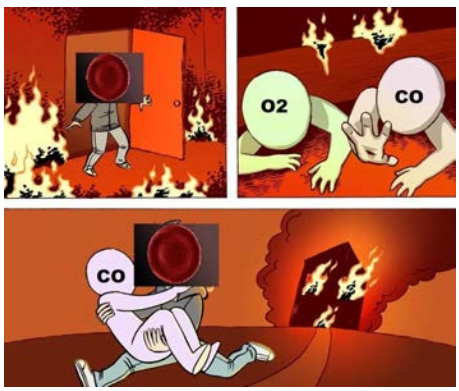


Cartoon image of a generic zinc finger protein in which the green zinc is coordinated to 2 Cys ligands and 2 His ligands. Such proteins enforce specific protein folding, although the coordination spheres do vary. (Image from Wikipedia.)

Topics to Be Covered* (Chapter Numbers are from Kaim)

- **Chapter 1:** Historical Background, Current Relevance, and Perspectives
- **Chapter 2:** Some General Principles (review of coordination chemistry: nomenclature, Lewis acid-base theory, hard-soft acid-base theory, crystal/ligand field theory, etc.)
- **Physical Methods** (IR/Raman, NMR, EPR, Mössbauer, X-ray studies, and electrochemistry)
- **Chapter 3:** Cobalamins, Including Vitamin and Coenzyme B12 (bioorganometallics, general reactions, enzymatic functions, and model systems)
- **Chapter 5:** The Dioxygen Molecule, O_2 (properties of O_2, hemoglobin and myglobin, hemerythrin and hemocyanin)
- **Chapter 6:** Catalysis through Hemoproteins (cytochrome P450, peroxidases, oxygenases)
- **Chapter 7:** Iron-Sulfur and Other Non-heme Iron Proteins (rubredoxin, ferredoxin, ribonucleotide reductase, monooxygenase, phosphatases)
- **Chapter 8:** Uptake, Transport and Storage of Iron (siderophores, transport, and storage)
- **Chapter 9:** Nickel-containing enzymes (urease, hydrogenase, acetyl CoA Synthase, SOD)
- **Chapter 10:** Copper-containing proteins ("blue" copper proteins, cytochrome *c* oxidase)
- **Chapter 11:** Biological Functions of the "Early" Transition Metals: V, Mo, W, and Cr (oxotransferases, nitrogenases, haloperoxidases)
- **Chapter 12:** Zinc (carbonic anhydrase, hydrolases, ADH, "zinc finger" proteins)
- **Chapter 18:** Biochemical Behavior of Radionuclides and Medical Imaging
- **Chapter 19:** Chemotherapy Involving Nonessential Elements (cisplatin, gold arthritis drugs, lithium-based drugs, ulcer treatments, etc.)

*Due to time constraints, not all Chapters (or all sections of each Chapter) will be covered.



While it's a funny meme, it's not quite that simple. Simple heme iron complexes in solution show a ***significantly*** higher affinity for CO than O_2. However, in blood cells this affinity for CO is only slightly higher. This is why placing patients in hyperbaric (high pressure) O_2 chambers will help to release the CO by shifting the equilibrium.

Le Châtelier's Principle to the rescue!

Tentative Schedule

Dates (Thursdays)	Topic(s)	Assignments
Aug 29	Syllabus, Ch 1, Start Ch 2	In-class HW Ch 2
Sept 5	Continue Ch 2	In-class HW Ch 2, Ch 2 HW (tentative), Entatic State article
Sept 12	Finish Ch 2 (if needed), start Phys Methods	Ch 2 HW (if not assigned), Phys Methods in-class HW
Sept 19	Continue Physical Methods	More in-class Phys Methods HW
Sept 26	Finish Phys Methods	More in-class Phys Methods HW, Phys Meth HW
Oct 3	Ch 3, Ch 5	Ch 3 and Ch 5 reading/problem sets
Oct 10	Ch 6, Ch 7	Ch 6 and Ch 7 reading/problem sets
Oct 17	Exam 1	CHEM 5339 students only: have journal article for presentation approved
Oct 24	Ch 8, Ch 9	Ch 8 and Ch 9 reading/problem sets
Oct 31	Ch 10, Ch 11	Ch 10 and Ch 11 reading/problem sets
Nov 7	Ch 12	Ch 12 reading/problem sets
Nov 14	Ch 18/19	No assignment :)
Nov 21	Exam 2	Start working on presentation
Nov 28	Thanksgiving—No class!	Keep working on presentation, but also relax during the week off (if possible)!
Dec 5	Presentations, Part 1	
Dec 12	Presentations, Part 2	

University Policies and Information (Last Update – 5/30/2024)

WITHDRAWING FROM CLASS

Students may withdraw (drop) from this course using the Withdrawal Portal. Withdrawing (dropping) this course can impact your Financial Aid, Scholarships, Veteran Benefits, Exemptions, Waivers, International Student Status, housing, and degree progress. Please speak with your instructors, consider your options, speak with your advisor, and visit the One-Stop Service Center (STE 230) or email enroll@uttyler.edu to get a complete review of your student account and the possible impacts to withdrawing. We want you to make an informed decision. UT Tyler faculty and staff are here for you and often can provide additional support options or assistance. Make sure to carefully read the implications for withdrawing from a course and the instructions on using the Withdrawal portal.

Texas law prohibits students from dropping more than six courses during their entire undergraduate career.* The six courses dropped include those from other 2-year or 4-year Texas public colleges and universities. Consider the impact withdrawing from this class has on your academic progress and other areas, such as financial implications. We encourage you to consult your advisor(s) and Enrollment Services for additional guidance. CAUTION #1: Withdrawing before census day does not mean you get a full refund. Please see the Tuition and Fee Refund Schedule. CAUTION #2: All international students must check with the Office of International Programs before withdrawing. All international students are required to enroll full-time for fall and spring terms. CAUTION #3: All UT Tyler Athletes must check with the Athletic Academic Coordinator before withdrawing from a course. CAUTION #4: All veterans or military-affiliated students should consult with the Military and Veterans Success Center.

*Students who began college for the first time before 2007 are exempt from this law.

ARTIFICIAL INTELLIGENCE STATEMENT

UT Tyler is committed to exploring and using artificial intelligence (AI) tools as appropriate for the discipline and task undertaken. We encourage discussing AI tools' ethical, societal, philosophical, and disciplinary implications. All uses of AI should be acknowledged as this aligns with our commitment to honor and integrity, as noted in UT Tyler's Honor Code. Faculty and students must not use protected information, data, or copyrighted materials when using any AI tool. Additionally, users should be aware that AI tools rely on predictive models to generate content that may appear correct but is sometimes shown to be incomplete, inaccurate, taken without attribution from other sources, and/or biased. Consequently, an AI tool should not be considered a substitute for traditional approaches to research. You are ultimately responsible for the quality and content of the information you submit. Misusing AI tools that violate the guidelines specified for this course is considered a breach of academic integrity. The student will be subject to disciplinary actions as outlined in UT Tyler's Academic Integrity Policy. Refer to the About This Course section of the UT Tyler Syllabus Module for specific information on appropriate use of AI in your course(s), or see below.

For this course, you can use AI programs (ChatGPT, Copilot, etc.) for exam preparation (e.g., generating flashcards and sample test questions). Be aware that in cases where information provided by AI conflicts with the lecture material, the lecture material will take priority. You will NOT be permitted AI on exams. Remember, AI does make mistakes, so I recommend the "trust but verify" policy when it comes to using AI.

FINAL EXAM POLICY

Final examinations are administered as scheduled. If unusual circumstances require that special arrangements be made for an individual student or class, the Dean of the appropriate college, after consultation with the faculty member involved, may authorize an exception to the schedule. Faculty members must maintain student final examination papers for a minimum of three months following the examination date.

INCOMPLETE GRADE POLICY

If a student, because of extenuating circumstances, is unable to complete all the requirements for a course by the end of the semester, then the instructor may recommend an Incomplete (I) for the course. The "I" may be assigned in place of a grade only when all of the following conditions are met: (a) the student has been making satisfactory progress in the course; (b) the student is unable to complete all coursework or final exam due to unusual circumstances that are beyond personal control and are acceptable to the instructor, and (c) the student presents these reasons before the time that the final grade roster is due. The semester credit hours for an Incomplete will not be used to calculate the grade point average.

The student and the instructor must submit an Incomplete Form detailing the work required and the time by which the work must be completed to their respective department chair or college dean for approval. The time limit established must not exceed one year. Should the student fail to meet all the work for the course within the time limit, then the instructor may assign zeros to the unfinished work, compute the course average for the student, and assign the appropriate grade. If a grade has yet to be assigned within one year, then the Incomplete will be changed to an F, or NC. If the course was initially taken under the CR/NC grading basis, this may adversely affect the student's academic standing.

GRADE APPEAL POLICY

Disputes regarding grades must be initiated within sixty (60) days from the date of receiving the final course grade by filing a Grade Appeal Form with the instructor who assigned the grade. A grade appeal should be used when the student thinks the final course grade awarded does not reflect the grades earned on assessments or follow the grading scale as documented in the syllabus. The student should provide the rationale for the grade appeal and attach supporting document about the grades earned. The form should be sent via email to the faculty member who assigned the grade. The faculty member reviews the rationale and supporting documentation and completes the instruction section of the form. The instructor should return the form to the student, even if a grade change is made at this level. If the student is not satisfied with the decision, the student may appeal in writing to the Chairperson of the department from which the grade was issued. In situations where there is an allegation of capricious grading, discrimination, or unlawful actions, appeals may go beyond the Chairperson to the Dean or the Dean's designee of the college from which the grade was issued, with that decision being final. The Grade Appeal form is found in the Registrar's Form Library.

NOTE: The Grade Appeal Form is different from the Application for Appeal form submitted to the Student Appeals Committee, which does not rule on grade disputes as described in this policy.

University Policies and Information (cont.)

DISABILITY/ACCESSIBILITY SERVICES

In accordance with Section 504 of the Rehabilitation Act, Americans with Disabilities Act (ADA) and the ADA Amendments Act (ADAAA), the University of Texas at Tyler offers accommodations to students with learning, physical, and/or psychological disabilities. If you have a disability, including a non-visible diagnosis such as a learning disorder, chronic illness, TBI, PTSD, ADHD, or a history of modifications or accommodations in a previous educational environment, you are encouraged to visit https://hood.accessiblelearning.com/UTTyler/ and fill out the New Student application. The Student Accessibility and Resources (SAR) office will contact you when your application has been submitted and an appointment with the Assistant Director Student Accessibility and Resources/ADA Coordinator. For more information, including filling out an application for services, please visit the SAR webpage at https://www.uttyler.edu/disability-services, the SAR office located in the Robert Muntz Library, LIB 460, email saroffice@uttyler.edu, or call 903.566.7079.

MILITARY AFFILIATED STUDENTS

UT Tyler honors the service and sacrifices of our military-affiliated students. If you are a student who is a veteran, on active duty, in the reserves or National Guard, or a military spouse or dependent, please stay in contact with your faculty member if any aspect of your present or prior service or family situation makes it difficult for you to fulfill the requirements of a course or creates disruption in your academic progress. It is important to make your faculty member aware of any complications as far in advance as possible. Your faculty member is willing to work with you and, if needed, put you in contact with university staff who are trained to assist you. The Military and Veterans Success Center (MVSC) has campus resources for military-affiliated students. The MVSC can be reached at MVSC@uttyler.edu or via phone at 903.565.5972.

STUDENTS ON AN F-1 VISA

To remain in compliance with Federal Regulations requirements you must do the following:

- Traditional face-to-face classes: Attend classes on the regular meeting days/times.
- Hybrid Classes: Attend all face-to-face classes convened by the instructor according to the schedule set for your specific course.
- Online course: Only one online course can count toward your full-time enrollment. Students are expected to be fully engaged and meet all requirements for the online course.

ACADEMIC HONESTY AND ACADEMIC MISCONDUCT

The UT Tyler community comes together to pledge that "Honor and integrity will not allow me to lie, cheat, or steal, nor to accept the actions of those who do." Therefore, we enforce the Student Conduct and Discipline policy in the Student Manual Of Operating Procedures (Section 8).

FERPA

UT Tyler follows the Family Educational Rights and Privacy Act (FERPA) as noted in University Policy 5.2.3. The course instructor will follow all requirements to protect your confidential information.

ABSENCE FOR OFFICIAL UNIVERSITY EVENTS OR ACTIVITIES

This course follows the practices related to Excused Absences for University Events or Activities as noted in the Catalog.

ABSENCE FOR RELIGIOUS HOLIDAYS

This course follows the practices related to Excused Absences for Religious Holy Days as noted in the Catalog.

ABSENCE FOR PREGNANT STUDENTS

This course follows the requirements of Texas Laws SB 412, SB 459, SB 597/HB 1361 to meet the needs of pregnant and parenting students. Part of the supports afforded pregnant students includes excused absences. Faculty who are informed by a student of needing this support should make a referral to the Parenting Student Liaison. NOTE: Students must work with the Parenting Student Liaison in order to receive these supports. Students should reach out to the Parenting Student Liaison at parents@uttyler.edu and also complete the Pregnant and Parenting Self-Reporting Form.

CAMPUS CARRY

We respect the right and privacy of students who are duly licensed to carry concealed weapons in this class. License holders are expected to behave responsibly and keep a handgun secure and concealed. More information is available at http://www.uttyler.edu/about/campus-carry/index.php.