Bioinorganic Chemistry

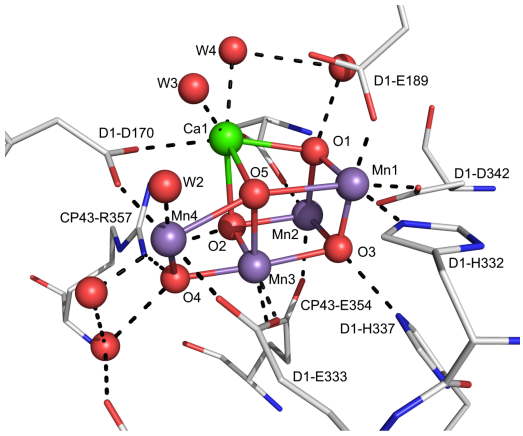
SECTION (CRN): 446-001 (73504)
LECTURE: TR 9:00-10:15am, Robinson Hall A412
PREREQUISITES: CHEM 332, CHEM 337 with grade of C or better

COURSE DESCRIPTION

CHEM 446 - Bioinorganic Chemistry
Application of inorganic coordination chemistry and physical methods in study of structure and function of metal ion sites in biomolecules. Properties of transition metal ions, ligand field theory. Topics include iron cytochromes, zinc and copper enzymes, cobalamins, iron sulfur proteins, oxygen transport, iron storage, electron transfer, inorganic model compounds, metals in medicine, and toxicity of inorganic species.

INSTRUCTOR

Rebecca M. Jones, Ph.D.
Term Associate Professor
Department of Chemistry and Biochemistry
STEM Accelerator, College of Science
Phone: (703) 993-1084
Email: rjones22@gmu.edu
Office: Exploratory Hall 1402
Office Hours: M 10:30am-11:45am, T 2:45-3:30pm, or by appointment



X-ray Crystal structure of the Mn_4O_5Ca core of the oxygen-evolving complex of Photosystem II

REQUIRED TEXTS

Inorganic Chemistry, 5th Edition *(earlier editions acceptable)*
by Gary L. Miessler, Paul J. Fischer, Donald A. Tarr, Prentice Hall, 2014
(ISBN-13: 978-0321811059, ISBN-10: 0321811054)

Bioinorganic Chemistry
Dieter Rehder, Oxford University Press, 2014
(ISBN: 9780199655199)

STUDENT RESPONSIBILITY

Successful completion of this course requires attendance at all lectures sessions. If you are absent from a normal class period, you are responsible for all the material covered. If you are involved in a university activity and will miss an exam session, you must contact the professor at least one week in advance to schedule a make-up time. An absence will be excused only if the instructor is notified in advance (e.g. before 9:00am on the day of the absence) and suitable documentation is provided to explain (e.g. a doctor's note). No make-up exams for unexcused absences will be given.

Students are responsible for all course changes during the semester; changes will be announced in class and by email to students' university email address.

ATTENDANCE

Successful completion of this course requires attendance at all lecture periods. If you are absent from a normal class period, you are responsible for all the material covered. If you are involved in a university activity and will miss a class in which an exam will be given, you must contact the professor at least one week in advance to schedule a make-up time. An absence will be excused only if the instructor is notified in advance (e.g. before 8:00am on the day of the absence) and suitable documentation is provided to explain (e.g. a doctor's note). No make-up exams or quizzes for unexcused absences will be given.

EVALUATION

Students will be assigned a grade based upon three types of assessments; assignments, midterm exams and a cumulative final exam. Recommended problems from the end of each chapter are listed in the attached lecture schedule.

EXAMS

Exam dates are shown in the attached class schedule. Approved calculators will be allowed; no cell phones or other mobile devices may be used. All exams and quizzes require that you show your work; assume that all questions say 'explain' or 'show calculations'. Often, the numerical answer will not be worth the full point value of the question. Partial credit will be awarded in appropriate situations.

Evaluation			
Method	**Number**	**Value**	**Total**
Assignments			
Point Group Worksheet	1	50	50
Infographic Assignment	1	50	50
Rehder Chapter summaries	5	10	50
Midterm Exams	2	100	200
Final Exam	1	150	150
		Total	**500 pts**

Total Points	**Grade**
450-500	A- / A / A+
388-449	B- / B / B+
325-387	C / C+
263-324	D
1-262	F

LECTURE SCHEDULE

Week	*Day*	*Date*	*Topic*	*End of Chapter Problems*
1	T	29-Aug	Chapter 1 (Miesslar): Intro and Syllabus	
	Th	31-Aug	Chapter 2: Atomic Structure	*Miesslar: 2-4, 15-17, 19-23, 26, 29, 33, 36, 42, 43, 46*
2	T	5-Sep		
	Th	7-Sep		
3	T	12-Sep	Chapter 3: Simple Bonding Models	*Miesslar: 2-4, 6, 8-11, 13, 16, 17, 20, 21, 26, 29*
	Th	14-Sep		
4	T	19-Sep	Chapter 4: Symmetry	*Miesslar: 1, 2, 3, 4, 5, 6, 6, 8, 9, 12a, 13a*
	Th	21-Sep		
5	T	26-Sep		
	Th	28-Sep	**Exam 1** (Ch. 1-4)	*Point group worksheet due in class*
6	T	3-Oct	Chapter 5: Molecular Orbitals	*Miesslar: 2, 3, 4, 5, 8*
	Th	5-Oct		
7	T	10-Oct	**No Classes – Monday classes meet**	
	Th	12-Oct	Chapter 6: Acid/Base Chemistry	*Miesslar: 1, 10, 15, 20, 21*
8	T	17-Oct	*In Chapter Exercises*	*Miesslar: 6-1, 6-3, 6-4*
	Th	19-Oct	Chapter 9: Intro to Coordination Chem	*Miesslar: 1, 2, 3, 4, 5, 12, 13*
9	T	24-Oct		***Infographic first-draft due - Bb***
	Th	26-Oct	Chapter 10: Coordination Chem	*Miesslar: 1, 2, 9, 11, 12, 13, 15a, 20, 21*
10	T	31-Oct		
	Th	2-Nov		
11	T	7-Nov	**Exam 2** (Ch. 5, 6, 9, 10)	
	Th	9-Nov	Chapter 1 (Rehder): Intro to bioinorganic	
12	T	14-Nov	Chapter 4-5: Iron, Oxygen transport	
	Th	16-Nov		
13	T	21-Nov	Chapter 6: Oxidoreductases	
	Th	23-Nov	**No Classes – Thanksgiving Break**	
14	T	28-Nov	Chapter 11: Photosynthesis	
	Th	30-Nov		
15	T	5-Dec	Chapter 14: Inorganics in medicine	
	Th	7-Dec	Final Exam Review	***Infographic Final Assignment Due***
Finals	Th	14-Dec	**Cumulative Final Exam** (7:30am-10:15pm)	

CHEM 446
Bioinorganic Chemistry
Lecture Topics

Atomic Structure (Chapter 2)

- Review atomic spectra, quantum numbers, atomic orbitals and electron configurations
- Coulombic energy and Exchange energy related to Hund's rule
- Calculating effective nuclear charge (Slater's rules)
- Periodic trends: electronegativity, ionization energy, atomic and ionic radii

Simple Bonding Theory (Chapter 3)

- Review Lewis structures, VSEPR geometries, formal charge, molecular polarity
- Using formal charge to choose best resonance structure
- Lone pair and bonded pair repulsion, explanation of VSEPR geometries
- Electronegativity and atomic size effects on bond angles and lengths

Symmetry (Chapter 4)

- Symmetry Elements and operations
- Assigning point groups

MO Theory (Chapter 5)

- MOs from s, p, d orbitals
- Symmetry considerations for formation
- MO diagrams for homonuclear and heteronuclear diatomics
- *Polar bonds, predicting bonds for heteronuclear diatomics*

Acid-Base and Donor-Acceptor Chemistry (Chapter 6)

- Frontier orbitals and acid-base reactions
- Hard-soft acid-base theory (HSAB), predicting solubility and interactions

Coordination Chem I: Structure and Isomers (Chapter 9)

- Define coordination sphere, ligand, chelates, etc.
- Example molecules of different coordination numbers

Coordination Chem II- Bonding (Chapter 10)

- Magnetic susceptibility, calculating spin-only
- Intro Valence Bond and Xtal field theory briefly
- Detailed presentation of Ligand Field Theory, focus on d-orbital splitting
- High-spin vs. low-spin, calculation spin-only moments for complexes
- Spectrochemical series
- Understanding exchange energy and coulombic energy's roles in electronic structure.
- Formation of complex MOs, sigma and pi bonding
- Different geometries: octahedral, *square planar, and tetrahedral*

Bioinorganic topics (Rehder Text)

- The various roles of metals in biological systems
- Oxygen transport, oxidoreductases, photosynthesis
- Metals in medicine

ACADEMIC INTEGRITY

Students are expected to conduct themselves appropriately at all times. Disruptive students who refuse to cooperate will be asked to leave the class session and may be removed from the course. Disruptive behavior may be defined, but is not limited to, any activities that disturb the learning environment including disrespectful outbursts, offensive language, and the use of any electronic or other device that interrupts the concentration of others. Cell phones, pagers, etc. must be turned off or silenced for the duration of class.

Mason has an Honor Code with clear guidelines regarding academic integrity. Three fundamental and rather simple principles to follow at all times are that: (1) all work submitted be your own; (2) when using the work or ideas of others, including fellow students, give full credit through accurate citations; and (3) if you are uncertain about the ground rules on a particular assignment, ask for clarification. No grade is important enough to justify academic misconduct.

Academic and classroom misconduct will not be tolerated. Academic dishonesty may be defined as any act of dishonesty in academic work. This includes, but is not limited to, plagiarism, the changing or falsifying of any academic documents or materials, cheating, and giving or receiving of unauthorized aid in tests, examinations, or other assigned work. Students guilty of academic misconduct, either directly or indirectly through participation or assistance, are immediately responsible to the instructor of the class. The penalty for cheating will be a grade of "F" on the work in question; at the instructor's discretion, the incident may be referred to academic affairs for disciplinary action.

DIVERSITY

George Mason University promotes a living and learning environment for outstanding growth and productivity among its students, faculty and staff. Through its curriculum, programs, policies, procedures, services and resources, Mason strives to maintain a quality environment for work, study and personal growth.

PRIVACY

Students must use their University email account to receive important University information, including messages related to this project. See http://masonlive.gmu.edu for more information.

DISABILITY ACCOMMODATIONS

If you are a student with a disability and you need academic accommodations, please see me and contact the Office of Disability Services (ODS) at 703-993-2474, http://ods.gmu.edu. All academic accommodations must be arranged through the ODS.

A PERSONAL NOTE

Inorganic chemistry is a very diverse and interesting subject! I want you to succeed in this class and will do all I can to help you do well. Completing assigned problems and keeping on schedule with lecture will positively influence your grade. Asking questions is very encouraged both in lecture and lab. Best wishes for your success this semester!

This syllabus is tentative and subject to change at the instructor's discretion.