Chemistry 616: Physical Inorganic Chemistry – Electronic Structure and Spectroscopy (Winter 2018)

Professor: Nicolai Lehnert; 2807 Chem
Office Hours: By Appointment, email: lehnertn@umich.edu, phone: 615-3673
Class Hours: Tuesday, Thursday, 10.00 am – 11.30 am, 1624 CHEM

	Topic	Assigned Reading
Jan 04	General Considerations: electromagnetic radiation, nature and energy of light, lifetime	Introductory textbooks to physical chemistry
Jan 09	General Considerations (cont.): lifetime and bandshape	Introductory textbooks to physical chemistry
Jan 11	Electronic Absorption Spectroscopy: the interaction of matter with light, QM treatment	
Jan 16	Einstein coefficients, Integrated Absorption: the Lambert-Beer Law	Introductory textbooks to physical chemistry
Jan 18	Ligand Field Transitions: fundamental concepts of orbitals & states	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Jan 23	The Pauli Principle and the antisymmetric wave function, atomic states	
Jan 25	Ligand Field Transitions (cont.): Atomic states, Tanabe-Sugano Diagrams, electronic selection rules	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Jan 30	Ligand Field Transitions (cont.): Franck-Condon principle, vibronic coupling	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 01	Ligand Field Transitions (cont.): vibronic coupling	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 06	Charge-Transfer Transitions: Franck-Condon factors	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 08	Electron Paramagnetic Resonance (EPR): angular and spin momentum, the Zeeman effect	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 13	EPR (cont.): the S = ½ system, g shifts and anisotropy, spin-orbit coupling	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 15	The S = ½ system (cont.)	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 20	Hyperfine coupling: coupling of electron and nuclear spins	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 22	The Spin Hamiltonian: application and case studies	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 06	EPR (cont.): spin systems with S > ½, zero-field splitting	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 08	The Spin Hamiltonian (cont.): spin systems with S > ½, zero-field splitting	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 13	Magnetic Circular Dichroism (MCD): the Stevens equation, A, B, C terms	Johnson in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 15	MCD (cont.): S = ½ systems, the MCD selection rules, types of MCD intensity	Johnson in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 20	Touring the EPR facility and practical demonstrations (**with Jim Windak**)	Please meet at the EPR room: 4709 CHEM
Mar 22	MCD (cont.): spin systems with S > ½, saturation curves and electronic polarizations, case studies	Johnson in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 27	Normal Coordinate Analysis (NCA): vibrational analysis, multidimensional harmonic oscillator, the g and f matrix, symmetrization, case study: water	Chemical Applications of Group Theory (Cotton)
Mar 29	Resonance Raman Spectroscopy: classical treatment, QM scattering equation	Spiro in: Physical Methods in Bioinorganic Chemistry (Que)

	Topic	Assigned Reading
Apr 03	Resonance Raman Spectroscopy (cont.): vibronic coupling, the A, B, C terms, the resonance Raman effect, case studies: [Fe(TPP)(Cl)] and Cytochrome P450cam	Spiro in: Physical Methods in Bioinorganic Chemistry (Que)
Apr 05	Mössbauer Spectroscopy	Handout
Apr 10*	X-ray Crystallography workshop, part 01	
Apr 12*	X-ray Crystallography workshop, part 02	
Apr 17*	X-ray Crystallography workshop, hands-on	

* The X-ray Crystallography workshop will be directed by our librarian, **Dr. Yulia Sevryugina**, who has in-depth experience in this topic from her Ph.D. and postdoctoral work.

Preparation: If you would like to prepare for the class, and refresh the basics of spectroscopy, the following book is recommended:

Inorganic Spectroscopic Methods; Brisdon, A. K.; Oxford Chemistry Primers, Vol. 62, Oxford University Press, New York, 2000

Requirements: Your grade will be based on the homework and two exams.

Exam 1 (Date and Location TBA)	30% of final grade
Final Exam (Date and Location TBA)	30% of final grade
Homework (9 problem sets + workshop)	40% of final grade

NOTE: If you will not be able to attend an exam ***for any reason,*** you must notify Professor Lehnert ***before*** the exam takes place. You will *not* be able to take a make-up exam unless this policy is followed.

Textbooks: Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism; Que, L., ed.; University Science Books, Sausalito, CA, 2000

Other Resources:

- Handouts
- Inorganic Electronic Structure and Spectroscopy Part I & II (Solomon, Lever)
- Physical Methods in Chemistry (Drago); unfortunately out of print, but maybe available in the library
- Chemical Applications of Group Theory (Cotton)
- Molecular Vibrations (Wilson, Decius, Cross)
- Modern Quantum Chemistry (Szabo, Ostlund)
- Quantum Mechanics in Chemistry (Simons, Nichols)

Grievance policy:
Departmental policy indicates the first step in inquiring about the accuracy of a final grade should be directed to the lead instructor of the course. This initial inquiry should take place within the first fifteen University business days of the first full term following the term in which the disputed grade was issued. If, after this inquiry, the student is not satisfied with the instructor's response, the student may choose to initiate a formal grade grievance. To initiate a formal grade grievance, the student should contact the Associate Chair of Undergraduate Studies (ACUS) of the home department of the course in question before the end of the fifth week of classes in the first full term following the term in which the disputed grade was issued.