Chemistry 616: Physical Inorganic Chemistry – Electronic Structure and Spectroscopy (Winter 2022)

Professor: Nicolai Lehnert; 2807 Chem
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Class Hours: Tuesday, Thursday, 10.00 am – 11.30 am, 1624 CHEM

	Topic	Assigned Reading
Jan 06	General Considerations: electromagnetic radiation, nature and energy of light, lifetime and bandshape	Introductory textbooks to physical chemistry
Jan 11	General Considerations (cont.): lifetime and bandshape	
Jan 13	Electronic Absorption Spectroscopy: the interaction of matter with light, QM treatment	
Jan 18	Einstein coefficients, Integrated Absorption: the Lambert-Beer Law	Introductory textbooks to physical chemistry
Jan 20	Ligand Field Transitions: fundamental concepts of orbitals & states	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Jan 25	The Pauli principle and the antisymmetric wave function, atomic states	
Jan 27	Ligand Field Transitions (cont.): Atomic states, Tanabe-Sugano Diagrams, electronic selection rules	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb. 01	Ligand Field Transitions (cont.): Franck-Condon principle, vibronic coupling	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb. 03	Ligand Field Transitions (cont.): Vibronic coupling	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 08	Charge-Transfer Transitions: Franck-Condon factors	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 10	Electron Paramagnetic Resonance (EPR): angular and spin momentum, the Zeeman effect	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 15	EPR (cont.): the S = ½ system, g shifts and anisotropy, spin-orbit coupling	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 17	The S = ½ system (cont.)	McMillin in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 22	The Spin Hamiltonian: application and case studies	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Feb 24	Hyperfine coupling: coupling of electron and nuclear spins	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 08	EPR (cont.): spin systems with S > ½, zero-field splitting	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 10	The Spin Hamiltonian (cont.): spin systems with S > ½, zero-field splitting	Palmer in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 15	Magnetic Circular Dichroism (MCD): the Stevens equation, A, B, C terms	Johnson in: Physical Methods in Bioinorganic Chemistry (Que)
Mar 17	MCD (cont.): S = ½ systems, the MCD selection rules, types of MCD intensity	Johnson in: Physical Methods in Bioinorganic Chemistry (Que)
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 24	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	X-ray absorption spectroscopy *	
Mar 31	X-ray absorption spectroscopy (cont.) *	
Apr 05	Resonance Raman Spectroscopy: classical treatment, QM scattering equation	Spiro in: Physical Methods in Bioinorganic Chemistry (Que)
Apr 07	Resonance Raman Spectroscopy (cont.): vibronic coupling, the A, B, C terms, the resonance Raman effect	Spiro in: Physical Methods in Bioinorganic Chemistry (Que)

	Topic	Assigned Reading
Apr 12	Resonance Raman Spectroscopy (cont.): case studies: [Fe(TPP)(Cl)] and Cytochrome P450cam	Handout
Apr 14	Mössbauer Spectroscopy	Handout
Apr. 19	Mössbauer Spectroscopy (cont.) and Nuclear Resonance Vibrational Spectroscopy	Handout

* Guest lecture by Prof. Jim Penner-Hahn

Preparation: In order to prepare for the class, **you should refresh on quantum mechanics (!)** and the basics of spectroscopy. In the latter case, 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)	40% of final grade

Homework sets and other materials will be distributed via the Canvas course site.

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.