Instructor

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Lecture

TR 10:05 – 11:20 AM, Votey 223

Office Hours

MW 10:00 AM – 11:00 AM, Discovery W112

Exams

March 21, 10:05 – 11:05 AM, Votey 223
May 7, 1:30 – 2:30 PM, Votey 223

Course Description

Determination of molecular and electronic structure of inorganic complexes using spectroscopic techniques. Introduction to magnetism. Interpretation of spectroscopic data within the frameworks of group theory and electronic structure calculations.

Textbook

Required: Que, Lawrence Jr. *Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism*, University Science Books, 2000.

Recommended: Cramer, C.J. *Essentials of Computational Chemistry*, Wiley, 2004.
Miessler, G.L.; Fischer, P.J.; Tarr, D.A. *Inorganic Chemistry*, Pearson, 2014.

Web Content

Lecture notes will be available through Blackboard (bb.uvm.edu). These materials are available for all current, UVM-affiliated, students, but they may not be shared off-campus without permission of the instructor.

Course Goals

Upon completion of Chem 236, it is anticipated that you will:

1. Identify appropriate physical characterization tool(s) for an inorganic species of interest.
2. Describe the sample and instrumentation requirements for these techniques.
3. Analyze spectroscopic data using group theory and electronic structure calculations.
4. Understand physical characterizations of inorganic species described in the literature.

Academic Honesty

As UVM students, you are expected to conduct yourself in accordance with the Code of Academic Integrity: http://www.uvm.edu/policies/student/acadintegrity.pdf

Our Common Ground

As UVM students, you are expected to conduct yourself in accordance with Our Common Ground: http://www.uvm.edu/~presdent/?Page=miscellaneous/commonground.html

Course Schedule

Jan. 15: Course Introduction
Jan. 17: Molecular Orbitals (MF&T 5.3, 10.3-10.4)
Jan. 22: Electronic States (MF&T 10.3-10.5, 11.2)
Jan. 24: Density Functional Theory (Cramer 8.1-8.3)
Jan. 29: ***NO CLASS***
Jan. 31: ***NO CLASS***
Feb. 5: Exchange-Correlation Functionals (Cramer 8.4)
Feb. 7: Electronic Absorption Spectroscopy (Que 1.1-1.8), ***PS #1 Due***
Feb. 12: Charge Transfer Transitions (Que 1.9-1.11)
Feb. 14: Ligand Field Transitions (Que 1.12-1.17)
Feb. 19: Time-dependent DFT (Cramer 14.1-14.3)
Feb. 21: IR and Raman Spectroscopy (Que 2.1-2.2), ***PS #2 Due***
Feb. 26: Molecular Vibrations (Que 2.3)
Feb. 28: Resonance Enhancement (Que 2.4)
Mar. 5: ***NO CLASS***
Mar. 7: Frequency Calculations (Cramer 9.3)
Mar. 12: ***NO CLASS***
Mar. 14: ***NO CLASS***
Mar. 19: Spin-orbit Coupling (Que 3.1-3.2A), ***PS #3 Due***
Mar. 21: ***Exam #1***
Mar. 26: Spin-spin Coupling (Que 3.2B-3.2F)
Mar. 28: Hyperfine Coupling (Que 3.3)
Apr. 2: Coupled-Perturbed Self-Consistent Field Calculations (Cramer 9.1)
Apr. 4: Circular Dichroism (CD) Spectroscopy (Que 5.1-5.7), ***PS #4 Due***
Apr. 9: Magnetic CD Spectroscopy (MCD) (Que 5.8-5.9A)
Apr. 11: Variable-temperature, variable-field MCD (Que 5.9B-5.11)
Apr. 16: Complete-active space Self-Consistent Field Calculations (Cramer 7.1-7.4)
Apr. 18: Hyperfine Shift (Que 8.1A-8.1B), ***PS #5 Due***
Apr. 23: Paramagnetic Relaxation (Que 8.1C-8.1D)
Apr. 25: Two-dimensional NMR Spectroscopy (Que 8.2)
April 30: NMR Resonance Assignment Strategies
May 2: Course Evaluations, ***PS #6 Due***
May 7: ***Exam #2***

Grading

Exams (67%): Two one-hour exams are scheduled for Chem 236. These exams are *not* cumulative.

Problem Sets (33%): A total of 6 open-book, open-notes problem sets will be assigned throughout the semester. Problem sets are due at **10:00 AM** on the due date. Late Problem sets will not be accepted, but the lowest score will be dropped.