

**Instructor**

Prof. Matt Liptak  
Discovery W112  
(802) 656 – 0161  
[matthew.liptak@uvm.edu](mailto:matthew.liptak@uvm.edu)

**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>

*The instructor reserves the right to change everything, with notice*

### 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.

*The instructor reserves the right to change everything, with notice*