**CHEM 5494**
**Special Topics in Inorganic Chemistry: Spectroscopic Methods in Inorganic Chemistry**


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| Instructor: | Dr. Stephen M. Holmes | Course Time: | 5:30 – 6:45 MW |
| Office Location: | 418 Benton Hall | Course Location: | 451 Benton Hall |
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| Office Hours: | Wed. 2-3 PM and by appointment | | |


**Suggested Texts**:

A. Vincent, *Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Ed.*; John Wiley & Sons: New York, 2001.

A. K. Brisdon, *Inorganic Spectroscopic Methods*; Oxford University Press: New York, 1998.

S. Ducket; B. Gilbert, *Foundations of Spectroscopy*; Oxford University Press: New York, 2000.

J. A. Iggo, *NMR Spectroscopy in Inorganic Chemistry*; Oxford University Press: New York, 2003.

**Supplementary Texts** (optional/useful references for your library):

E. A. V. Ebsworth; D. W. H. Rankin; S. Cradock, *Structural Methods in Inorganic Chemistry, 2nd Ed.* (currently out of print).

R. S. Drago, *Physical Methods for Chemists, 2nd Ed.* (math-heavy)

K. Nakamoto, *Infrared and Raman Spectra of Inorganic Coordination Compounds*; 5th Ed.

J. E. Wertz; J. R. Bolton, *Electron Spin Resonance*

J. B. Lambert; H. F. Shurvell; D. Lightner; R. G. Cooks, *Introduction to Organic Spectroscopy*

H. Friebolin, *Basic One- and Two-Dimensional NMR Spectroscopy*; 2nd Ed.

C. N. Banwell, *Fundamentals of Molecular Spectroscopy*; 3rd Ed.

A. F. Orchard, *Magnetochemistry*

**Grading Distribution**

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|---|---|---|---|
| 60% | Exams (3 x 20%) | 15% | Homework (5 x 3%) |
| 5% | Wiki Module Project | 20% | Final Exam (comprehensive) |

**Fall 2008** **CHEM 5494**

**Special Topics in Inorganic Chemistry: Spectroscopic Methods in Inorganic Chemistry**

| | Date | Tentative Topics |
|---|---|---|
| Mon. | Aug. 18 | Introduction and Basics of Molecular Symmetry |
| Wed. | Aug. 20 | Molecular Symmetry and Group Theory: Symmetry operations and elements |
| Mon. | Aug. 25 | Symmetry transformations and Mulliken symbols |
| Wed. | Aug. 27 | Basic Infrared spectroscopy and selection rules |
| *Mon.* | *Sept. 1* | *Academic holiday* |
| Wed. | Sept. 3 | Introduction to X-ray crystallography (N. Rath) ***Homework 1 Due (in class)*** |
| Mon. | Sept. 8 | X-ray crystallography in inorganic chemistry (N. Rath) |
| Wed. | Sept. 10 | Group Theory: IR and Raman |
| Mon. | Sept. 15 | Infrared spectroscopy continued |
| Wed. | Sept. 17 | Raman spectroscopy: Introduction |
| Mon. | Sept. 22 | Raman spectroscopy; Examples ***Homework 2 Due (in class)*** |
| Wed. | Sept. 24 | ***EXAM 1 (5:30-6:45)*** |
| Mon. | Sept. 29 | Nuclear Magnetic Resonance Spectroscopy (NMR): Basics & Chemical Shift Origins (spin-spin splitting, chemical shift equivalence, magnetic equivalence) |
| Wed.. | Oct. 1 | NMR: CSE, ME, tree diagrams for coupling interactions |
| Mon. | Oct. 6 | NMR: Factors impacting $J_{x,y}$ coupling, relaxation mechanisms |
| Wed. | Oct. 8 | NMR: spin systems, virtual coupling, and examples ***Homework 3 Due (in class)*** |
| Mon. | Oct. 13 | Magnetism and magnetic susceptibility basics |
| Wed. | Oct. 15 | Magnetism: Term Symbols, States, Magnetic field-dependence |
| Mon. | Oct. 20 | Magnetism: Molecule-based systems |
| Wed. | Oct. 22 | Electron Paramagnetic Resonance: Theory and examples |
| Mon. | Oct. 27 | Electron Paramagnetic Resonance, Mössbauer Spectroscopy ***Homework 4 Due (in class)*** |
| Wed. | Oct. 29 | ***EXAM 2 (5:30-6:45)*** |
| Mon. | Nov. 3 | Electronic Spectroscopy: UV-visible Spectroscopy Basics & UV-vis Selection rules, Spectrochemical, and Neuphelauxetic Series |
| Wed. | Nov. 5 | UV-vis Spectroscopy: Calculation of $D_q$, $\beta$, Orgel and Tanabe-Sugano diagrams |
| Mon. | Nov. 10 | UV-vis examples and discussion |
| Wed. | Nov. 12 | Mass Spectrometry: Ionization techniques and mechanisms |
| Mon. | Nov. 17 | Mass Spectrometry: Fragmentation mechanisms |
| Wed. | Nov. 19 | Mass Spectrometry: Functional group fragmentation ***Homework 5 Due (in class)*** |
| *Mon.* | *Nov. 24* | *Fall Break, Academic Holiday* |
| *Wed.* | *Nov. 26* | *Fall Break, Academic Holiday* |
| Mon. | Dec. 1 | Catch-up day and Wiki Module |
| ***Wed.*** | ***Dec. 3*** | ***EXAM 3 (5:30-6:45)*** |
| ***Fri.*** | ***Dec. 5*** | ***Wiki Spectroscopy Module (Due at 12 AM)*** |
| ***Mon.*** | ***Dec. 8*** | ***FINAL EXAM (5:30-7:30)*** |