

Daniel R. Gamelin Department of Chemistry University of Washington Autumn, 2003

# **Chemistry 508**

### **Advanced Inorganic Chemistry**

Autumn, 2003

Instructor:	Professor Daniel Gamelin
	CHB 204K, 685-0901
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Lectures: Monday, Wednesday, Friday, 9:30-10:20, Bagley 106

**Office Hours:** By appointment

**Prerequisites:** Assumes some familiarity with quantum mechanics and statistical thermodynamics

#### **Suggested Text Books:**

Drago: Physical Methods in Chemistry, 2nd Edition Cotton: Chemical Applications of Group Theory, 3rd Edition

Reserve Texts (Chemistry Library):

Ballhausen: Introduction to Ligand Field Theory Hitchman and Figgis: Ligand Field Theory and its Applications Nakamoto: Infrared and Raman Spectra of Inorganic and Coordination Compounds Cotton: Chemical Applications of Group Theory

Grading:	Problem sets (approx. 6)	40% total
	Take-home exams (3)	60% total

**Problem Sets:** All problem sets must be completed to pass this class. They will be graded on a pass/fail basis.

**Exams**: All exams must be completed to pass this class. Exams should reflect an individual effort and will be graded accordingly.

**Exam and HW policy:** You are strongly encouraged to work with other students on both HW and exams. You may use any books for assistance, but the work you turn in should be your own. The honor code requires that you do not use previous 508 exams, HW, etc.!

### **Tentative Exam Dates:**

#1. Friday, Oct. 10	(Due in class, Friday, Oct. 17)
#2. Wednesday, Nov. 19	(Due in class, Wednesday, Nov. 26)
#3. Wednesday, Dec. 10	(Due before 10:20AM, Tuesday, Dec. 16, 2003)

## **Tentative Sequence of Lecture Topics**

### Part A. Molecular Symmetries and Molecular Vibrations

- 1. Symmetry elements, groups, point groups
- 2. Representations of groups, character tables
- 3. Matrix representation of symmetry operations, direct products
- 4. Reducible representations, molecular vibrations
- 5. Internal and symmetry coordinates, symmetry adapted linear combinations (SALCs)
- 6. Polyatomic molecular vibrations, degeneracies, orbital SALCs
- 7. Vibrational spectroscopy, selection rules for IR absorption
- 8. Selection rules for Raman spectroscopy, depolarization effects
- 9. Normal coordinate analysis, the GF matrix method

### Part B. Electronic Structures and Spectroscopies of Transition-Metal Ions

- 10. Molecular orbital theory: diatomics
- 11. Molecular orbital theory: coordination complexes, absorption spectroscopy
- 12. Crystal field theory
- 13. Multiple electrons: strong-field limit
- 14. Multiple electrons: weak-field limit
- 15. Correlation diagrams, Tanabe-Sugano diagrams, Ligand field theory
- 16. Properties of Tanabe-Sugano diagrams
- 17. Ligand-field electronic absorption spectroscopy
- 18. Spin selection rule and spin-orbit coupling
- 19. Low symmetry effects in ligand-field electronic absorption spectra
- 20. Polarized absorption spectroscopy
- 21. Artificial discontinuities, spin-crossover compounds, and the LIESST effect
- 22. Excited-state distortions and electronic absorption bandshapes
- 23. Radiative and nonradiative excited-state relaxation processes
- 24. Luminescence spectroscopy, transition-metal lasers

### Part C. Magnetism and Magnetic Ground States of Transition-Metal Ions

- 25. Magnetism and magnetic properties of transition metal ions
- 26. Orbital angular momentum in magnetism
- 27. Electron paramagnetic resonance (EPR) spectroscopy: high symmetry
- 28. EPR spectroscopy: low symmetry and Jahn-Teller effects
- 29. Magnetic exchange coupling in transition-metal dimers
- 30. Orbital basis for magnetic exchange interactions