\[ Q = E_a(+) \]
\[ \frac{1}{2\sqrt{3}} \left( 2\Delta r_1 - \Delta r_2 - \Delta r_3 + 2\Delta r_4 - \Delta r_5 - \Delta r_6 \right) \]

(axial)

\[ \text{Absorbance [a.u.]} \]

\[ \text{Emission intensity [a.u.]} \]

\[ \text{Energy [cm}^{-1}\text{]} \]

\[ \text{ZnO band gap} \]

\[ \text{Absorption [a.u.]} \]

\[ \text{Co}^{2+} \]

\[ 4T_1(P) \]

\[ \sigma_{V}(3) \]

\[ x' \quad y' \quad x \]

\[ M \quad L \]

\[ \begin{array}{c}
\text{ML} \\
\text{2500} \\
\text{2000} \\
\text{1500} \\
\text{3000} \\
\text{2500} \\
\text{2000} \\
\text{1500} \\
\end{array} \]

\[ \text{Energy [cm}^{-1}\text{]} \]

\[ \begin{array}{c}
1S \\
1A_{1g} \\
1G \quad 1E_{g} \quad 1T_{1g} \quad 1T_{2g} \\
3P \\
3F \quad 3A_{2g} \quad 3T_{2g} \quad 3T_{1g} \\
\end{array} \]

\[ \text{Weak Field Limit} \]

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
Gamelin@chem.washington.edu

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:
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