Chemistry 634
Physical Methods in Inorganic Chemistry

Instructor: Dr. Timothy Hughbanks
Time: TTh 9:35 - 10:50 PM; Room 2101
Office Hours: Tuesday 2:00 - 4:00. Other times are OK too, as available

Texts (loosely followed):
C. Hammond, "The Basics of Crystallography and Diffraction";
J. Iggo, "NMR Spectroscopy in Inorganic Chemistry";
A. F. Orchard, "Magnetochemistry";
Harris & Bertolucci, "Symmetry and Spectroscopy, An Introduction to Vibrational and Electronic Spectroscopy".

The course will provide an introduction to methods of determining of molecular and crystal structures and physical properties of inorganic compounds. Because this is a survey course, a single textbook that adequately discusses all topics covered is difficult to identify. Students are especially encouraged to read from the broader readings in the attached reading list and to identify other sources for themselves.

The grades will be based on the homework (≤40%), midterm and final exams (≥60%). The anticipated point breakdown should go as follows: ~4-5 problem sets (160-200 pts total), one-hour exam (100 pts), and a final exam (200 pts). You are expected to make a serious attempt at every assigned homework problem before consulting with your peers, otherwise collaboration is permitted as long as significant contributions are made by all collaborators. Do not expect to be able to do all problems in a problem set in a single sitting.

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Course Outline

I. X-ray Diffraction and Space Groups *~ 4-5 weeks*

A. Lattices and Space Groups
Bravais lattices
Plane Groups
Space Groups – "simple" symmorphic cases w/examples
Structures vs lattices
Glide Planes and screw axes w/examples
Survey of examples of space groups applied to structures

B. Reciprocal lattices and Diffraction
Mathematical definition of reciprocal lattices
and geometric relationships to direct (Bravais) lattices
Role of reciprocal lattice in diffraction
– the condition for constructive interference
Fraunhofer diffraction vs. Bragg/Laue diffraction – an optical analogy
Structure factors
Systematic Absences and symmetry

C. A Conceptual walk through 'typical' crystal structure determinations
Data collection
Unit cell and symmetry
Intensities
Data Reduction
Structure Solution
Finishing Touches

II. Electronic Structure and Spectroscopy of TM Complexes *~ 2-3 weeks*

A. MO Theory
Ligand Field Theory
Valence Bond Theory (deficiencies of elementary approach)

B. Ligand Effects; Metal Effects
σ-donors
π-donors
π-acceptors
Metal-dependent trends

C. Electronic States of TM complexes
d-d transitions; connecting atomic states and molecular states
High-spin and low-spin molecules
Jahn-Teller effects - applications of subgroups
Selection rules for electronic transitions in molecules
LMCT and MLCT transitions
Aspects of solid-state spectroscopy

III. EPR Spectroscopy~ *2-3 weeks*

A. Background
   What is EPR?
   Electronic Structure of Atoms and open-shell ions
   Spin-Orbit Coupling
   g-values in atoms
   Zeeman interaction

B. Hyperfine coupling
   Connection to wavefunctions
   Simple radicals
   Hyperfine anisotropy – dipolar contributions
   Complex cases

C. The *g*-tensor
   Phenomenological meaning of g-values
   Why are *g*-values anisotropic in molecules?
   Relationship between *g*-tensor, "fictitious" spin, and "true" spin
   Spin-orbit coupling, electronic structure, and *g*-value anisotropy
   Examples

IV. Magnetism ~ *2 weeks*

A. Phenomenological survey
   Ideal paramagnets (Curie Law) and weakly interacting paramagnets (Curie-Weiss)
   Ferromagnets, antiferromagnets, and ferrimagnets
   Basics of magnetic measurements

B. Mechanisms of magnetic coupling
   Coupling in dimers
   Magnetostructural correlations – whether by design or by discovery

V. Nuclear Magnetic Resonance Spectroscopy ~ *2 weeks*

A. Fundamentals
   Energy levels, transitions, sensitivity issues, timescales
   Chemical shielding and shifts, basics and a few advanced ideas
   Spin-spin coupling and decoupling
   Basics of relaxation and the vector model

B. Structure Determination
   Trends in chemical shifts
   Factors influencing coupling constants
   Chemical and magnetic equivalence
   First- and second-order spectra
   Relaxation and structure

C. Other topics
   Dynamic processes
   NMR of paramagnetic compounds

Chemistry 634 - Other Suggested Books

Author(s), Editors	Title
Abragam & Bleaney	Electron Paramagnetic Resonance of Transition Ions
Brisdon	Inorganic Spectroscopic Methods
Canet	Nuclear Magnetic Resonance Concepts and Methods
Carrington & McLachlan	Introduction to Magnetic Resonance
Cheetham & Day	Solid-State Chemistry Techniques
Clegg	Crystal Structure Determination
Cotton	Chemical Applications of Group Theory, 3rd Edition
Drago	Physical Methods for Chemists, 2nd Edition
Eberhart	Structural and Chemical Analysis of Materials
Ebsworth, Rankin & Cradock	Structural Methods In Inorganic Chemistry, 2nd Ed.
Friebolin	Basic One-and Two-Dimensional NMR Spectroscopy
Orchard	Magnetochemistry
Orton	Electron Paramagnetic Resonance
Giacovazzo, Monaco, Viterbo, Scordari, Gilli, Zanotti, Catti	Fundamentals of Crystallography
Solomon & Lever, eds.	Inorganic Electronic Structure and Spectroscopy, Volumes I & II
Stout & Jensen	X-Ray Structure Determination-A Practical Guide
Wertz & Bolton	Electron Spin Resonance
Weltner	Magnetic Atoms and Molecules