

CHEM 634: Physical Methods in Inorganic Chemistry

Spring 2011 SYLLABUS

Tuesday and Thursday: 11:10 am - 12:25 pm, CHAN 2122

INSTRUCTOR: Professor Janet Bluemel—Reed McDonald building (RMD), room 323 (via 321)
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OFFICE HOURS: T/Th 12:30 pm-2:30 pm; other times available by appointment

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TEXTBOOKS:

- [1] Analytical Chemistry. Editors R. Kellner, J.-M. Mermet, M. Otto, H. M. Widmer, Wiley-VCH, 1998, 1st Edition.
ISBN: 3-527-28881-3 (paperback)
- [2] Techniques in Inorganic Chemistry. Editors J. P. Fackler, Jr., L. R. Falvello, CRC Press, 2011, 1st Edition.
ISBN: 978-1-4398-1514-4 (hardback)
- [3] Basic One- and Two-Dimensional NMR Spectroscopy. H. Friebolin, Wiley-VCH, 2005, 4th Edition.
ISBN: 3-527-31233-1 (paperback)

Because this is a survey course, a single textbook that adequately discusses all topics covered is difficult to identify. Therefore, the students will be provided with course material (lecture and exercise material), and the powerpoint files.

COURSE GRADING:

Exam I (Feb. 22, 2011, CHAN 2122)	20 %
Exam II (March 22, 2011, CHAN 2122)	30 %
Final Exam: Friday, May 6, 2011, from 3:00 pm - 5:00 pm (CHAN 2122)	50 %

There will be two written exams during the course, and one written final exam at the end of the course. The students are also welcome to bring research problems from their own graduate projects for discussion, or give short presentations themselves.

COURSE DESCRIPTION and LEARNING GOALS:

My aim is to provide a contemporary introduction to the diverse and fascinating spectroscopic techniques available today for determining the molecular and crystal structures, as well as physical properties of inorganic compounds and materials. These inorganic species display a wide range of characteristics, and they include, for example, solids, liquids and gases. Although this variety and diversity are intrinsic features of inorganic chemistry, there are underlying patterns and trends which can be used to identify the most favorable physical methods to analyze and properly describe a given inorganic molecule or material.

My goal is to provide all students (a) with an insight into the most powerful spectroscopic techniques, and (b) with a solid foundation on which to build understanding. At the end of the course all students should be able to deal with analytical challenges that might arise in their research, and identify and apply the proper techniques that solve the problems unequivocally and quickly. Achievements in recent research, as well as industrial aspects, will be included in this course. Examples from publications and seminar talks presented by visitors during the semester will be discussed.

COURSE OUTLINE (Topics **II, III, VI,** and **VII** follow the outline in textbook [1])

I. NMR Spectroscopy of Liquids and Solids

- (1) The Basics of one- and two-dimensional NMR Spectroscopy
 - the NMR experiment and the main features of the NMR spectrometer
 - the chemical shift and proper referencing with internal and external standards
 - the J -coupling and standard correlation spectroscopy
 - processing NMR spectra
- (2) Multinuclear and organometallic NMR spectroscopy
 - the more common spin-1/2 nuclei, e.g. ^{19}F , ^{31}P , ^{29}Si , ^{119}Sn
 - quadrupolar nuclei, e.g. ^2H , ^6Li , ^{11}B , ^{14}N , and their characteristics and applications
- (3) NMR of diamagnetic and paramagnetic organometallic compounds
 - peculiarities of $^1\text{H}/^{13}\text{C}$ chemical shifts
 - different J -coupling scenarios and virtual couplings
 - dynamic effects and ligand exchange
- (4) Interactions in the solid state and technical requirements of the spectrometer
 - Chemical Shift Anisotropy (CSA) and Magic Angle Spinning (MAS)
 - dipolar interactions and Cross Polarization (CP)
 - quadrupolar interactions

II. IR and Raman Spectroscopy

III. UV-VIS Spectroscopy, Emission and Luminescence

IV. ESR Spectroscopy of Liquids and Solids

- (1) Background
 - Zeeman interaction
 - Spin-orbit coupling
 - g -values in atoms
- (2) Hyperfine coupling
 - Simple radicals
 - Hyperfine anisotropy - dipolar contributions
- (3) The g -tensor
 - Anisotropy of g -values in molecules
 - g -tensor and spin
 - Spin-orbit coupling, electronic structure, and g -value anisotropy

V. Magnetism

- (1) Overview
 - Paramagnets, ideal (Curie Law), and weakly interacting (Curie-Weiss)
 - Ferromagnets, antiferromagnets, ferrimagnets
 - Magnetic Measurements
- (2) Mechanisms of magnetic coupling
 - Coupling in dimers
 - Magnetostructural correlations

VI. X-Ray and Neutron Powder and Crystal Diffraction

VII. Mößbauer Spectroscopy

The Americans with Disabilities Act (ADA) is a federal antidiscrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you believe you have a disability requiring an accommodation, please contact the Department of Student Life, Services for Students with Disabilities in Cain Hall, Rm. B118, or call 845-1637.

"An Aggie does not lie, cheat or steal, or tolerate those who do."