# Special Topic in Inorganic Chemistry: Spectroscopic Methods in Inorganic Chemistry CHEM 395 Spring 2015

## **Course Description:**

This is an upper level undergraduate or graduate course. The aim of this course is to provide students with a broad understanding of the spectroscopic methods that are available to identify structures of inorganic compounds (some techniques can also be applied for identification of organic compounds). The methods include NMR, EPR, vibrational, electronic and photoelectron, and Mössbauer spectroscopy, diffraction methods, and mass spectrometry. Specifics of instrumental design will be covered but the emphasis will be placed on the experimental methods and interpretation of spectra.

Instructor: Wei-Tsung Lee, office FH 402, telephone (773)508-3205.

Time and Location: Monday and Wednesday, 5:45–7:00 pm, FH 105

Office Hours: Tuesday and Wednesday 4:00-5:00 pm or by appointment.

### Reference Materials (Handouts will be provided):

*Organic Structural Spectroscopy*, J. B. Lambert, S. Gronnert, H. F. Shurvell, D. A. Lightner, and R. G. Cooks, Prentice Hall; 2nd edition, 2010.

Inorganic Spectroscopic Methods, A. K. Brisdon, Oxford University Press; 1998.

*Electronic and Photoelectron Spectroscopy: Fundamentals and Case Studies*, A. M. Ellis, M. Feher, and T, G. Wright, Cambridge University Press; Reissue edition, 2011.

Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth, D. W. H. Rankin, and S. Cradock, Blackwell; 2nd edition, 1991.

#### Grading:

Grading will be based on homework assignments (approximately one per week) (25%), one midterm exam (20%), a final exam (30%) and a presentation (25%). On homework assignments, two or three randomly selected problems will be graded, but the solutions to all the problems will be posted after the assignment is due.

#### Homework Assignments:

Assignments relevant to the material presented in class will be given each class. Many questions will come from the above textbooks as well as other ones. Special emphasis will be placed on interpretation of spectra.

#### **Presentation/Hands-on Example:**

Each student will give a 20–30 minute presentation on a spectroscopic or spectrometric method of analysis from the literature or a hands-on example. The method can be an advanced application of the methods discussed in class or a method that has not been covered in class. The presentation will include theory, example of spectra or data, discussion of how data is obtained and processed, discussion of how data is interpreted to solve a chemical problem. The hands-on

example can be one that is readily performed by you in your research projects. Students are especially encouraged to develop an application that is new and especially make use of instruments in our department (mass spectrometry, NMR, and EPR spectroscopy).

Week (estimate)	Topics	Content
1	NMR Spectroscopy	Theory, Instrument Design, 1-D
		Experiment, Interpretation of Spectra
2	NMR Spectroscopy	2-D Experiments and Interpretation of
		Spectra
		Information from Coupling Constants
3	NMR Spectroscopy	Relaxation, Solid and Paramagnetic
		Compounds, Monitoring Reactions
4	EPR Spectroscopy	Theory, Instrumentation, Interpretation of
		Spectra, Nuclear Quadrupole Resonance
		(NQR) Experiment
5	Rotational Spectroscopy	Theory, Instrument Design, Selection
		Rules
		Interpretation of Spectra
6	Vibrational Spectroscopy	Theory, Instrument Design, Vibrational
		Spectra and Symmetry
		Assignment of Bands to Vibrations
7	Vibrational Spectroscopy	Fingerprints, Use of Isotopes in
		Interpreting Vibrational Spectra
		Resonance Raman Spectroscopy
8	Midterm Exam	
9	Electronic and Photoelectron	Theory, Instrumentation, Electronic
	Spectroscopy	Spectroscopy, Interpretation of Spectra
10	Electronic and Photoelectron	Photoelectron Spectroscopy, Circular
	Spectroscopy	Dichroism
11	Mössbauer Spectroscopy	Theory, Instrumentation, Parameters
		from Mössbauer Spectra
12	Diffraction Methods	Theory, Instrument Design, Power and
		Single Crystal Diffraction
13	Mass Spectrometry	Theory, Instrument Design, Overview of
		Spectra
14	Case Studies	Comprehensive Case Studies from
		Lectures
15	Case Studies	Comprehensive Case Studies from

Topics and Approximate Schedule:

		Lectures
16	Student Presentation	
17	Student Presentation	
18	Final Exam	