CHEMISTRY
Fall 2009

CHEM 521: Advanced Organic Chemistry I Menger/Padwa MTWT 1:00-2:15
Content: This course will cover the principles of physical organic chemistry starting with bonding theory, structure, thermochemistry and kinetics. These basic principles will be integrated into a mechanistic description of organic reactions. Techniques for describing, understanding and analyzing reaction mechanisms will be presented ("arrow-pushing", energy profiles, isotope effects, solvent effects, stereochemical and conformational analysis). Prerequisites are organic chemistry and physical chemistry.
Texts: Advanced Organic Chemistry--Part A-4th edition -Carey and Sundberg
Max: 30

CHEM 522: Advanced Organic Chemistry II Davies MWF 8:30-9:45
Content: The course begins with brief overview of the principles of organic synthesis (e.g., retrosynthetic analysis, selectivity, symmetry, convergence). This is followed by a survey of organic reactions beginning with a description of the fundamental reactions and reactivity patterns of carbonyl compounds and olefins. Other reactions are then presented in the context of how they are to be applied to the synthesis of organic molecules. Specific topics include: stereoselective olefin synthesis; pericyclic reactions; small and medium ring synthesis; acyclic stereocontrol; and asymmetric synthesis. Stereochemistry and chirality are extensively illustrated through the examination of stereoselective organic reactions. Prerequisite Chem 221-222 (or equivalent introductory organic course).
Texts Required: Modern Physical Organic Chemistry (Anslyn, Dougherty), University Science Books, ISBN 1-891389-31-9 and Strategic Applications of Named Reactions in Organic Synthesis (Kurti and Czako), Elsevier, ISBN 0-12-429785-4
Max: 18

CHEM 531: Intro Moleculular Quantum Mechanics Bowman TT 11:30-12:45
Content: This course will present the foundations of modern quantum chemistry. The Schroedinger equation and applications to a variety of one, two and three dimensional problems will be presented. The necessary background of special functions and basics of quantum mechanics will also be presented.
Texts: N/A
Max: 19

CHEM 535: Physical Methods in Experimental Chem Widicus Weaver MW 10:00-11:15
Content: This course will provide an introduction to the experimental techniques of modern physical chemistry. It will cover theoretical and practical issues pertaining to equipment (including lasers, optical elements, and detectors) as well as experimental design.
Texts: N/A
Max: 19

536 Kindt TT 10:00-11:15

Advanced Physical Chemistry V

Introduction to the statistical basis of thermodynamics, and its application to systems including molecular gases, liquids, metals, semiconductors, polymers, and the Bose-Einstein condensate. Foundations of molecular dynamics and Monte Carlo simulation methods.

Textbook: Understanding Molecular Simulations: From Algorithms to Applications" by Berend Smit and Daan Frenkel.

Max: 19

CHEM 551: Adv Inorganic Chemistry MacBeth TT 11:30-12:45

Content: Advanced inorganic chemistry will cover basic coordination chemistry and Group Theory and its application to inorganic chemistry. We will survey the chemistry of inorganic compounds from the standpoint of chemical bonding principles. We will learn to use molecular orbital theory to describe the structure and reactivity of inorganic and organometallic complexes.

Texts: Principles of Structure and Reactivity (4th Edition) by Huheey, Keiter, Keiter

Texts (recommended):

Chemical Applications of Group Theory by Cotton

Advanced Inorganic Chemistry by Cotton

Particulars: Students will be evaluated using problem sets, examinations and one in class presentation.

Max: 18

CHEM 606: Ethics in Science Eisen

Content: Values in Science (IBS/Chem 606) is an intensive two-day course in research ethics sponsored and coordinated by the Graduate School of Arts and Sciences and the Center for Ethics. Values in Science is offered prior to both the Fall and Spring semesters on the dates listed below. The course satisfies the ethics training requirements of the National Institutes of Health and is designed for graduate students, post-doctoral fellows and others interested in addressing the objectives listed in the syllabus below.

CHEM 571: Spec Topics: BioMolecular Chemistry Lutz TT 10:00-11:15

Content: This course will focus on the chemistry and biology of nucleic acids and proteins. Following a review of the structural and functional properties of the building blocks of life, topics that will be discussed include: fundamentals of catalysis, catalytic nucleic acid, protein structure/function, protein folding and dynamics, as well as macromolecular machines (secondary metabolism).

Texts: N/A

Max: 18

575 Conticello MW 10:30-11:45

Content: The course involves the application of physical chemical approaches to study biological macromolecules in solution. Hydrodymanic (thermodynamic), spectroscopic, and kinetic approaches to understand biological structure and function of biological

macromolecules will be covered in the course.
Suggested Reference Texts (on reserve in Chemistry library):
Tanford, C. " Physical Chemistry of Macromolecules", J. Wiley & Sons, 1961
Cantor & Schimmel "Biophysical Chemistry" Parts I, II,& III, W.H. Freeman & Co. 1980.
Van Holde, K. et al. "Physical Biochemistry" Prentice-Hall, Inc. 2006
Campbell & Dwek "Biological Spectroscopy" Benjamin/Cummings Publ. Co. 1984
Laskowicz " Principles of Fluorescence Spectroscopy" Plenum Press, 1984
Cornish-Bowden "Fundamentals of Enzyme Kinetics" Portland Press, 2004 (3rd Ed.)
PREREQUISITES: Undergraduate Physical Chemistry (required); Undergraduate Biochemistry (Recommended)
GRADES: Are compiled from the results of two take-home exams, class participation on take home problems sets and the final exam is a student presentation on a topic related to the course materials.

729 Padwa/Menger TT 10:00-11:15
Special Topics in Organic Chemistry: Physical Organic
Chem 729 will include special topics in physical organic chemistry including classical organic kinetics studies, solvent effects, substituent effects, intermolecular forces, general acid/base catalysis etc.

752 Hagen TT 2:30-3:45
The objective of the course is to prepare students obtain crystal structures to support their research and to critically evaluate crystal structures (either their own as determined in house or published structures). Theory and practice of crystal design growth (ie Crystal Engineering). The course will cover practical and theoretical aspects of X-ray crystallography using the diffractometer and computer programs available in the Chemistry Department. Emphasis will be placed on the structure determination of small molecules by single crystal diffraction, but powder diffraction will also be covered. Students will carry out the structure determination of molecules from different research groups. Final reports in a format suitable for submission to a scientific journal will be expected.
Symmetry in two and three dimensions. Crystal morphology - face indexing. X-rays and Diffraction, Cell determination (recognizing twinning). Data collection. Space group determination. Structure solution and refinement. Analysis of crystal packing, bond lengths and angles. Preparation of figures and publishable reports.

Software: SHELXTL, CrystalMaker, CrystalDiffract, Single Crystal, WinGX, Platon, EnCIFer, PublCIF.

599 Kindt
Thesis Research

791 Lutz M 4:15-5:15
Analytical/Biomolecular Seminar

792 Inorganic Seminar	MacBeth	Tu 4:00-5:15
793 Organic Seminar	Blakey	W 2:30-3:45
794 Physical Seminar	Bowman	M 3:00-4:15
797 Directed Study	Kindt	
798 Research and Evaluation in Chemistry	Kindt	
799 Advanced Thesis Research	Kindt	