CHEMISTRY

Sterling Chemistry Laboratory, 203.432.3913
http://chem.yale.edu
M.S., Ph.D.

Chair
Kurt Zilm (chemistry.chair@yale.edu)

Director of Graduate Studies
Jonathan Ellman (jonathan.ellman@yale.edu)

Professors  Victor Batista, Gary Brudvig, Robert Crabtree, Craig Crews,* R. James Cross, Jr. (Emeritus), Jonathan Ellman, John Faller (Emeritus), Sharon Hammes-Schiffer, Nilay Hazari, Seth Herzon, Patrick Holland, Mark Johnson, William Jorgensen, J. Patrick Loria, James Mayer, J. Michael McBride (Emeritus), Scott Miller, Peter Moore (Emeritus), Anna Pyle,* James Rothman,* Martin Saunders, Charles Schmuttenmaer, Dieter Söll,* David Spiegel, Scott Strobel,* John Tully (Emeritus), Patrick Vaccaro, Elsa Yan, Frederick Ziegler (Emeritus), Kurt Zilm

Associate Professors  Jason Crawford, Timothy Newhouse

Assistant Professors  Caitlin Davis, Ziad Ganim, Stavroula Hatzios,* Sarah Slavoff, Hailiang Wang

Lecturers  Paul Anastas, Paul Cooper, Christine DiMeglio, Narasimhan Ganapathi, Jonathan Parr

* A secondary appointment with primary affiliation in another department.

FIELDS OF STUDY
Fields include bio-inorganic chemistry, bio-organic chemistry, biophysical chemistry, chemical biology, chemical physics, inorganic chemistry, materials chemistry, organic chemistry, physical chemistry, physical-inorganic chemistry, physical-organic chemistry, synthetic-organic chemistry, and theoretical chemistry.

SPECIAL REQUIREMENTS FOR THE PH.D. DEGREE
A foreign language is not required. Five term courses are required within the first two years of residence. Courses are chosen according to the student’s background and research area. To be admitted to candidacy a student must (1) receive at least two term grades of Honors, exclusive of those for research; (2) pass one oral examination—or, for biophysical chemistry students, two oral examinations—by the end of the second year of study; and (3) submit a thesis prospectus no later than the end of the third year of study. Remaining degree requirements include completing a formal independent proposal by the end of the fourth year, a written thesis describing the research, and an oral defense of the thesis. The ability to communicate scientific knowledge to others outside the specialized area is crucial to any career in chemistry. Therefore, all students are required to teach a minimum of two terms at a TF-20 level. Students who require additional support from the Graduate School must teach additional terms, if needed, after they have fulfilled the academic teaching requirement but will not be required to teach more than five terms over their first five years. All students are required to take CHEM 590, Ethical Conduct and Scientific Research, in the fall term of their first year of study.

MASTER’S DEGREE
M.S. (en route to the Ph.D.) A student must pass at least five graduate-level term courses in the Chemistry department exclusive of seminars and research. In addition, an overall average (exclusive of seminars and research) of High Pass must be maintained in all courses. One full year of residence is required.

Program materials are available online at https://chem.yale.edu/useful-links.

COURSES

CHEM 502a, Fundamentals of Transition Metal Chemistry  Patrick Holland
This half-term course covers the structures and properties of coordination compounds, and strategies for the design and analysis of new compounds. Elements of chelating ligands, spectroscopic methods, and magnetism are addressed. Prerequisites: two terms of organic chemistry and one term of inorganic chemistry (CHEM 252 or equivalent). ½ Course cr

CHEM 503a, Fundamentals of Organometallic Chemistry  Robert Crabtree
A half-term survey of the main principles of organometallic chemistry that enable students to understand basic concepts in the field. It prepares students for CHEM 504, the second half of this course. Prerequisites: two terms of organic chemistry and one term of inorganic chemistry (CHEM 252) or equivalent experience. ½ Course cr

CHEM 504b, Applications of Organometallic Chemistry  Nilay Hazari
A half-term survey of the applications of organometallic chemistry demonstrating the range of areas where organometallic reactions are important. It builds on the knowledge learned in CHEM 503. Prerequisite: CHEM 503 or equivalent experience. ½ Course cr
<table>
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<tr>
<th>Course Code</th>
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<tr>
<td>CHEM 505a</td>
<td>Inorganic Reaction Mechanisms</td>
<td>Patrick Holland</td>
<td>This half-term course covers the fundamentals of kinetics and mechanisms used by coordination compounds and transition-metal catalysts, and features analysis of papers from the recent literature. Prerequisites: two terms of organic chemistry, one term of inorganic chemistry, and CHEM 502 or equivalent. ½ Course cr</td>
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<tr>
<td>CHEM 513b</td>
<td>Electronic Structure in Inorganic Chemistry</td>
<td>Patrick Holland</td>
<td>This course covers a number of methods for analyzing the electronic structure of coordination complexes of the transition metals. It features the use of density-functional theory (DFT) to gain quantitative insight into properties, and critical analysis of the results. Prerequisite: CHEM 502 or equivalent. ½ Course cr</td>
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<tr>
<td>CHEM 518a</td>
<td>Advanced Organic Chemistry</td>
<td>Scott Miller</td>
<td>Concise overview of structure, properties, thermodynamics, kinetics, reactions, and intermolecular interactions for organic molecular systems.</td>
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<tr>
<td>CHEM 521a</td>
<td>Chemical Biology</td>
<td>Jason Crawford and Sarah Slavoff</td>
<td>A one-term introduction to the origins and emerging frontiers of chemical biology. Discussion of the key molecular building blocks of biological systems and the history of macromolecular research in chemistry.</td>
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<tr>
<td>CHEM 522b</td>
<td>Chemical Biology II</td>
<td>Sarah Slavoff</td>
<td>A comprehensive introduction to the origins and emerging frontiers of chemical biology.</td>
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<tr>
<td>CHEM 523a</td>
<td>Synthetic Methods in Organic Chemistry</td>
<td>Jon Ellman</td>
<td>This course surveys practical methods in synthetic organic chemistry with an emphasis on learning how to acquire new information and understand chemical reactivity from a fundamental and mechanistic perspective. Memorization is deemphasized. Undergraduates are encouraged to enroll.</td>
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<tr>
<td>CHEM 525b</td>
<td>Spectroscopic Methods of Structure Determination</td>
<td>Martin Saunders</td>
<td>The background and use of spectroscopic methods emphasizing NMR in organic chemistry. The course includes the use of programs for simulating spin-spin coupling and rapid rearrangement reactions in NMR. All methods commonly used by organic chemists for determining molecular structures of species in solution, in the gas phase, and in solids are included.</td>
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<tr>
<td>CHEM 530a</td>
<td>Statistical Methods and Thermodynamics</td>
<td>Victor Batista</td>
<td>The fundamentals of statistical mechanics developed and used to elucidate gas phase and condensed phase behavior, as well as to establish a microscopic derivation of the postulates of thermodynamics. Topics include ensembles; Fermi, Bose, and Boltzmann statistics; density matrices; mean field theories; phase transitions; chemical reaction dynamics; time-correlation functions; Monte Carlo and molecular dynamics simulations.</td>
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<tr>
<td>CHEM 531b</td>
<td>Special Topics in Organic Chemistry</td>
<td>Jon Ellman and Timothy Newhouse</td>
<td>Current topics in organic chemistry.</td>
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<tr>
<td>CHEM 537a</td>
<td>Chemistry of Isotopes</td>
<td>Martin Saunders</td>
<td>Advanced applications of isotopes to chemical problems and the theory associated with them, including kinetic and equilibrium isotope effects, tracer applications, and dating.</td>
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<tr>
<td>CHEM 542b</td>
<td>Molecules and Radiation II</td>
<td>Staff</td>
<td>An extension of the material covered in CHEM 540 to atomic and molecular spectroscopy, including rotational, vibrational, and electronic spectroscopy, as well as an introduction to laser spectroscopy.</td>
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<td>CHEM 553b</td>
<td>Small Molecule X-ray Crystallography</td>
<td>Brandon Mercado</td>
<td>This course provides an introduction to small molecule crystallography. It covers both theoretical and applied concepts and includes hands-on experience on how to solve and refine the structure of small molecules.</td>
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<tr>
<td>CHEM 554b</td>
<td>Bio-Inorganic Chemistry</td>
<td>Gary Brudvig</td>
<td>An advanced introduction to biological inorganic chemistry. Important topics in metalloprotein chemistry are illustrated. Objective is to define and understand function in terms of structure. Topics include catalysis with and without electron transfer, and carbon, oxygen, and nitrogen metabolism.</td>
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<td>CHEM 562a</td>
<td>Biochemical Rates and Mechanisms</td>
<td>J Patrick Loria</td>
<td>An advanced treatment of enzymology. Topics include transition state theory and derivation of steady-state and pre-steady-state rate equations. The role of entropy and enthalpy in accelerating chemical reactions is considered, along with modern methods for the study of enzyme chemistry. These topics are supplemented with in-depth analysis of the primary literature.</td>
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CHEM 562La or b / PHYS 762a or b, Laboratory in Instrument Design and the Mechanical Arts  
Familiarization with modern machine shop practices and techniques. Use of basic metalworking machinery and instruction in techniques of precision measurement and properties of commonly used metals, alloys, and plastics.  
Prerequisite: CHEM 562L.
CHEM 565Lb, Introduction to Glass Blowing  Daryl Smith and Patrick Vaccaro
The course provides a basic introduction to the fabrication of scientific apparatus from glass. Topics covered include laboratory setup, the fundamental skills and techniques of glass blowing, the operation of glass fabrication equipment, and requisite safety procedures.

CHEM 570a, Quantum Chemistry  Sharon Hammes-Schiffer
The elements of quantum mechanics developed and illustrated with applications in chemistry and chemical physics.

CHEM 576a, Fundamentals for Physical Chemistry  Mark Johnson
This course reinforces the principles of physics that are most relevant to experimental and theoretical physical chemistry. These include classical electricity and magnetism (with emphasis on the nature of light and the interaction of light with matter), optics, lasers, angular momentum, and atomic structure, including the spin-orbit interaction. The basic theme of the course is to provide students with physical intuition that can bridge the observations of everyday experience to the abstract concepts required for the correct, quantum-mechanical description of atomic-scale phenomena. Prerequisites: two terms of undergraduate physical chemistry (CHEM 328 or CHEM 332, and CHEM 333; or equivalents); and physics course work covering classical mechanics and electrostatics. ½ Course cr

CHEM 577a, Optics and Optical Components in Physical Chemistry Research  Mark Johnson
This course provides an intuitive understanding of optics and optical components that are used in modern physical chemistry laboratories. Topics include the polarization state of light, methods to calculate transmission and reflection coefficients beyond Snell's law, nonlinear optics, ultrafast lasers, regenerative amplifiers, plasmonics, and Fourier transforms. Prerequisites: undergraduate physics (including mechanics and E&M) and undergraduate physical chemistry; CHEM 576 is highly recommended but not necessarily required. ½ Course cr

CHEM 584b, Machine Learning and Quantum Computing in Chemistry and Materials Science  Victor Batista
Machine learning and quantum computing have emerged as leading technologies of the twenty-first century and are expected to be increasingly applied to a wide variety of chemical and materials science challenges. This course introduces fundamental concepts of machine learning and quantum computing to chemists and materials science students through an overview of algorithms, computational methods, and applications. It is intended to empower students to engage with this emerging field and foster the growing field of artificial intelligence for accelerated scientific discoveries in the molecular and physical sciences. Prerequisites: introductory quantum mechanics and Python, or permission of the instructor. ½ Course cr

CHEM 585b, Protein NMR Spectroscopy  J Patrick Loria
A theoretical treatment of solution NMR spectroscopy with emphasis on applications to proteins and biological macromolecules. This includes classical and quantum mechanical descriptions of NMR, product operator formalism, multidimensional NMR, phase cycling, gradient selection, relaxation phenomena, and protein resonance assignments. Prerequisite: physical chemistry that includes quantum mechanics; calculus and linear algebra are recommended but not required. ½ Course cr

CHEM 586b, Quantitative Biochemical Imaging  Caitlin Davis
Theory of optical microscopy, imaging, and image analysis with emphasis on quantitative characterization of the structure, dynamics, and chemical reactions of proteins, nucleic acids, and other biopolymers. Topics include optics of microscope and image formation, interaction of light and matter, fluorescent probes and biosensors, digital image processing, modern approaches in light microscopy (including confocal and multiphoton), and a brief introduction to electron microscopy and scanning probe techniques. Prerequisite: physical chemistry that includes quantum mechanics; calculus and linear algebra are recommended but not required. ½ Course cr

CHEM 590a, Ethical Conduct and Scientific Research  Jonathan Parr
A survey of ethical questions relevant to the conduct of research in the sciences with particular emphasis on chemistry. A variety of issues, including plagiarism, the falsification of data, and financial malfeasance, are discussed, using as examples recent cases of misconduct by scientists. Enrollment is restricted to graduate students in chemistry. 0 Course cr

CHEM 600a or b, Research Seminar  Staff
Presentation of a student's research results to the student's adviser and fellow research group members. Extensive discussion and literature review are normally a part of the series.

CHEM 700a or b, Laboratory Rotation for First-Year Biophysical and Chemical Biology Graduate Students  Staff
A seminar series based on invited speakers in the general area of organic chemistry.

CHEM 720a and CHEM 721b, Current Topics in Organic Chemistry  Seth Herzon
A seminar series based on invited speakers in the areas of physical, inorganic, and biological chemistry.

CHEM 740a and CHEM 741b, Seminar in Chemical Biology  Jon Ellman
CHEM 750a and CHEM 751b, Biophysical Chemistry Seminar  Caitlin Davis
CHEM 760a and CHEM 761b, Seminar in Inorganic Chemistry  Nilay Hazari
CHEM 990a or b, Research  Staff
Individual research for Ph.D. degree candidates in the Department of Chemistry, under the direct supervision of one or more faculty members.