

INDIANA UNIVERSITY

University Graduate School
2005-2006
Academic Bulletin

Chemistry

College of Arts and Sciences
Bloomington

Chairperson

David Clemmer*

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Departmental URL

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Graduate Faculty

(An asterisk [*] denotes membership in the University Graduate School faculty with the endorsement to direct doctoral dissertations.)

Chancellors' Professor

George Ewing* (Emeritus)

Harry G. Day Chair

David R. Williams*

Robert and Marjorie Mann Chairs

David E. Clemmer*, Gary M. Hieftje, Martin Jarrold*

Linda and Jack Gill Chair

Richard D. DiMarchi*

Lilly Chemistry Alumni Chair

Milos Novotny*

Distinguished Professors

Kenneth G. Caulton*, Ernest Davidson* (Emeritus), Frank Gurd* (Emeritus), Gary M. Hieftje, Ronald Hites* (Public and Environmental Affairs), Milos V. Novotny*, Peter J. Ortoleva* (Geological Sciences), Charles S. Parmenter*, Victor E. Viola*

Herman T. Briscoe Professor

Dennis G. Peters*

Professors

Adam Allerhand* (Emeritus), Edward Bair* (Emeritus), Russell Bonham* (Emeritus), Ernest Campaigne* (Emeritus), Marvin Carmack* (Emeritus), Jack Crandall* (Emeritus), Harry Day* (Emeritus), Romualdo T. de Souza*, P. Andrew Evans*, Joseph Gajewski* (Emeritus), Stanley Hagstrom* (Emeritus, Computer Science), W. Terry Jenkins* (Emeritus, Biochemistry and Molecular Biology), Lawrence K. Montgomery*, Krishnan

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Raghavachari*, James P. Reilly*, John Richardson* (Emeritus) (Biochemistry), V. Jack Shiner Jr.* (Emeritus), Lee Todd* (Emeritus), Rupert Wentworth* (Emeritus), Theodore S. Widlanski*, Jeffery M. Zaleski*

Associate Professors

S. Christopher Jacobson*, Caroline Chick Jarrold*, Jeffrey N. Johnston*, Martha Gray Oakley*, Philip S. Stevens* (Atmospheric Chemistry), Martin J. Stone*, Faming Zhang

Senior Scientist

Lyudmila Bronstein, John Huffman*

Assistant Professors

Mu-Hyun Baik, Donald H. Burke, Bogdan G. Dragnea, Andrew L. Feig, Daniel J. Mindiola, Srinivasan S. Iyengar, Dongwhan Lee, Thomas J. Tolbert

Graduate Advisor

Chemistry Building C121 (812) 855-2069

Degrees Offered

Master of Science, Master of Arts for Teachers, and Doctor of Philosophy. The department also participates in the biochemistry, chemical physics, and molecular and cellular biology programs.

Fields of Study

Analytical, biological, inorganic, organic, and physical chemistry.

Special Department Requirements

(See also general University Graduate School requirements.)

Admission Requirements

Undergraduate degree in chemistry, physics, mathematics, or the biological sciences. Students with undergraduate degrees in other areas of the physical sciences or engineering are also encouraged to apply. Students are admitted to the program only with the approval of the Chemistry Graduate Admissions Committee.

Grades

At least a B (3.0) average in work for the advanced degree. Grades below C (2.0) are not counted toward the completion of degree requirements but will be counted in determining a student's grade point average.

Master of Science Degree

This degree may be conferred upon the holder of a bachelor's degree or master's degree in another discipline.

Course Requirements

These requirements are flexible and are planned and approved by the graduate committee. A minimum of 30 credit hours in chemistry are required. At least 9 credit hours of course work in the major field offered in fulfillment of the M.S. degree must be in courses numbered 500 or above (excluding thesis work).

Thesis

Required.

Master of Arts for Teachers Degree

The M.A.T. program permits a secondary school teacher with minimum training in chemistry to achieve certification for the teaching major in chemistry in the secondary school. Teachers already holding such certification may strengthen their training by taking advanced lecture and laboratory work in chemistry. Students with B.A. or B.S. degrees in chemistry, but with no education courses, may complete requirements for a secondary Indiana teaching certificate and strengthen their chemistry training.

Admission Requirements

Eighteen (18) credit hours of chemistry, including one semester each of general, quantitative, and organic chemistry. Deficiencies must be removed without graduate credit. Continuance in the program will depend upon the results received in courses taken during the first semester of summer in the program; alternatively, a qualifying examination may be administered after either one semester or one summer in the program.

General Requirements

A total of 36 credit hours, of which a minimum of 20 credit hours must be in courses in chemistry that carry graduate credit. A maximum of 6 credit hours of undergraduate courses may be applied toward the M.A.T. degree. For a student having an unusually strong undergraduate background in chemistry or biochemistry, e.g., a B.S. degree, some of the required 20 credit hours in advanced chemistry courses may be in other areas of science and mathematics, if approved in advance by the graduate advisor. A student completing the requirements for the M.A.T. degree in chemistry must also have met the requirements for certification for a teaching major in science in the secondary school. Consult Education Student Services (Wright Education Building 1064, [812] 856-8511) for details.

Lecture-Course Requirements

Twelve (12) credit hours, distributed as follows: 6 credit hours in one of the five fields listed above and 3 credit hours in each of two of the remaining four. Lecture courses may be selected from those at the 500 level or above and from any of the following undergraduate courses: analytical, A314, A318; biological, C481, C483, C484, C485; inorganic, C430; organic, C342, S342, C443; physical, C360, C361, S361, C362, S362, C460.

Laboratory-Course Requirements

Two (2) credit hours chosen so that the student's total background in advanced laboratory courses will include credit in three different fields. The following, and comparable courses taken elsewhere, will qualify: A315, C344, S344, C364, C437, P464, C487.

Electives

Additional courses in chemistry at the 400 level or above to give a total of at least 20 credit hours (including course work in the above two categories). Up to 16 credit hours in courses at the 300 level or above in mathematics, biological sciences, physical sciences, or education carrying graduate credit.

Final Examination

Either oral or written or both.

Master of Library Science/Master of Information Science Degree Information Specialist (Chemistry)

Offered by the School of Library and Information Science (SLIS). Students in this joint program receive the Master of Library Science degree or the Master of Information Science degree and are certified as information specialists in chemistry.

Admission Requirements

Bachelor's degree in chemistry or the equivalent.

Course Requirements: M.I.S.

Foundation and Specialization course requirements (15 credit hours) and as elective courses L570, L624, and additional courses to total at least 26 credit hours. Additional courses are to be chosen in consultation with advisors in SLIS and Chemistry to bring the total graduate credit hours to 42.

Course Requirements: M.L.S.

Foundation courses (15 credit hours) and as elective courses L570, L624, and additional SLIS courses to total at least 30 credit hours. The additional courses are to be chosen in consultation with advisors in SLIS and Chemistry to bring the total graduate credit hours to 36.

Doctor of Philosophy Degree

The program leading to the Ph.D. degree emphasizes the attainment of a high level of competency in a specialized area of chemistry, but also requires the development of broad knowledge and experience. By the time the degree is earned, the student should show promise of becoming a capable and independent investigator in chemistry. The major emphasis for the Ph.D. is on research while in residence on the Bloomington campus. Research should be the student's greatest challenge and the focus of the major portion of his or her energy. The student's attitude toward and progress in research is a most important factor in graduate committee decisions.

Course Requirements

A total of 90 credit hours, of which at least 24 credit hours must be in course work. Students may major in analytical, biological, inorganic, organic, or physical chemistry. Doctoral students majoring in a field of chemistry are required to complete a minimum of 12 credit hours of course work in that field, following a sequence of courses approved by their advisory committee.

A doctoral student in chemistry can choose to minor within the chemistry department or can elect to minor in some other department. In the latter case, the requirements are specified by the minor department. Students electing to minor within the department must complete a minimum of 6 credit hours in areas of chemistry other than the major area. The course work comprising an inside minor must be approved by the advisory committee.

All doctoral students in chemistry are required to enroll in C500 Introduction to Research during their first year of study.

Foreign-Language/Tool-Skill Requirement

The department has no formal foreign language or tool-skill requirement, but Ph.D. advisory committees may consider such courses essential for individual students.

Qualifying Examinations

To remain in good standing, students must take the chemistry review course during their third and fourth semester and present a literature seminar by the end of the second year. In the fifth semester, students meet with their advisory committees to review past performance in both the major and minor areas and to evaluate plans for completing the Ph.D. This review includes a seminar, written document, and oral examination. Current information concerning probation, termination, and reinstatement policies may be obtained from the departmental graduate office.

Final Examination

Usually oral, covering dissertation, major, and minors, and also a seminar describing the dissertation.

Ph.D. Minor in Chemistry

Students from other departments who wish to minor in chemistry must complete at least 6 credit hours of graduate course work in chemistry with an average of B (3.0) or above.

Courses

C315 Chemical Measurements Laboratory I (3 cr.)

C317 Equilibria and Electrochemistry (2 cr.)

C318 Spectrochemistry and Separations (2 cr.)

C335 Inorganic Chemistry Laboratory (1-3 cr.)

C341 Organic Chemistry I Lectures (3 cr.) N&M P: C117 or C106. Chemistry of carbon compounds.

Nomenclature; qualitative theory of valence; structure and reactions. Syntheses and reactions of major classes of monofunctional compounds. Credit not given for both C341 and S341.

C342 Organic Chemistry II Lectures

C343-C344 Organic Chemistry Laboratory I-II (2-2 cr.)

C360 Introductory Physical Chemistry (3 cr.) N&M P: C117 or C106; N330 strongly recommended, MATH M119, PHYS P201; or equivalents. Elements of thermodynamics, reaction kinetics, molecular quantum states and spectroscopy. For students not intending to specialize in physical sciences. Credit given only for C360, C361/C362, or S361/S362.

C361 Physical Chemistry of Bulk Matter (3 cr.) N&M P: C117 or C106; N330 strongly recommended, MATH M212 or M216, and PHYS P202 or P222. Thermodynamics laws, free energy and chemical potentials, gases and dilute solutions, phase transitions, colligative properties, chemical equilibria, ionic solutions, chemical kinetics and transport processes, current topics. Credit given for only one of the following: C361, S361, or C360. I Sem.

C362 Physical Chemistry of Molecules (3 cr.) N&M P: C117 or C106; N330 strongly recommended, MATH M212 or M216, and PHYS P202 or P222.

S362 Physical Chemistry of Molecules, Honors (3 cr.)

C364 Introduction to Basic Measurements (3 cr.)

C405 Principles of Chemistry (1-3 cr.) For teachers of high school chemistry; offered in summer session only. May be repeated.

C406 Lecture Demonstration Techniques in Chemistry (1-2 cr.) Nonmajors only.

C430 Inorganic Chemistry (3 cr.) P: C106 or C118, or S106 or S118, or N330 or S330, and C342 or S342. R: C362 Structure and bonding of inorganic compounds; survey of chemistry of non-metal and metal elements, coordination compounds, organometallic compounds, mechanism and reactions.

C460 Nuclear Chemistry (3 cr.)

C483 Biological Chemistry (3 cr.)

C484 Biomolecules and Catabolism (3 cr.)

C485 Biosynthesis and Physiology (3 cr.)

C500 Introduction to Research (2-6 cr.; 6 cr. max.) Objectives and techniques of chemical research.

Assignment to research problem to be completed during two semesters.

C501 Chemical Instrumentation (4 cr.) Electronics as applied to chemical instrumentation; design and construction of instruments used in chemical research, analysis, recording, and control; maintenance and practice in modification to meet special needs.

C502 Spectroscopic Methods in Inorganic Chemistry (3 cr.) P: C361. Chemical applications of group theory and the elucidation of structure and bonding in inorganic molecules and complexes by vibrational, nuclear magnetic resonance, Mossbauer and electronic absorption spectroscopy.

C503 Spectrometric Methods of Structure Determination (3 cr.) P: graduate standing. Elucidation of molecular structure utilizing IR, UV, and NMR spectroscopy, mass spectrometry, and other methods.

C506 Biogeochemistry (3 cr.) The formation and processing of organic material in natural environments. Microbiology of sediments. The global biogeochemical cycles of carbon, nitrogen, and sulfur. Geochemistry of organic materials. Organic geochemical evidence of evolutionary events.

C509 Special Laboratory Problems (1-5 cr.) Nonmajors only. P: 8 credit hours of chemistry toward graduate degree, consent of instructor. P or C: 500-level lecture course in research field. Participation in scientific research to gain understanding of its philosophy and techniques.

C511 Advanced Analytical Methods I (4 cr.) Theory and practice of analytical separation techniques and analytical spectroscopy; chromatographic methods of separation, fundamentals of gas and liquid chromatography, overview of spectroscopic instrumentation, atomic and molecular spectroscopy for analysis.

C512 Advanced Analytical Methods II (4 cr.) Theory and practice of electrochemical (potentiometric and voltammetric) methods of analysis; introduction to analytical chemistry of the elements and statistics for analytical chemistry.

C540 Advanced Organic Chemistry (3 cr.) P: C362 and C342. Valence and molecule structure, electronic interpretation of organic reactions, stereochemistry.

C543 Organic Reactions (3 cr.) Synthesis of organic compounds, degradation reactions, selected topics in organic reactions.

C561 Atomic and Molecular Quantum Theory (3 cr.) P: graduate standing or consent of instructor. Elements of quantum theory, solution of elementary problems with chemical applications, approximate methods, atomic structure, molecular symmetry and normal vibrations, the molecular orbital description of molecules.

C562 Computational Quantum Chemistry (3 cr.) P: C561 or consent of instructor. Electronic structure theory at the Hartree-Fock and semiempirical levels, computer calculations on elementary systems, elements of group theory and linear vector spaces, electron correlation, structure of potential surfaces.

C566 Molecular Optical Spectroscopy (3 cr.) P: C561 or consent of instructor. Interaction of radiation with matter. Spectroscopic probes of the rotational, vibrational, and electronic structure of molecules. Advanced laser methods.

C567 Chemical Statistical Mechanics (3 cr.) P: graduate standing or consent of instructor. Introduction to equilibrium and nonequilibrium many-body systems using ensemble techniques. Emphasis on molecular systems and systems undergoing chemical transformation or transport. Both qualitative and rigorous approaches.

C568 Advanced Statistical Mechanics (3 cr.) P: C567 or consent of instructor. Selected topics such as pair correlation functions in classical liquids, laser and reaction-transport, nonequilibrium phenomena, critical phenomena, reaction rates, condensed media, NMR, precipitation and polymer kinetics, Green's function methods, and computational methods.

C572 Computational Chemistry and Molecular Modeling (3 cr.) P: C571 or consent of instructor. Molecular modeling: computer models of molecules and their behavior in gas and condensed phases; implicit and explicit solvation models; quantum and molecular mechanics; search strategies for conformational analysis, geometry optimization methods; information content from Monte Carlo and molecular dynamics simulations. Statistics and chemometrics: multivariate statistics and experimental design, numerical methods, calibration and chemical analysis, optimization methods, artificial intelligence. Molecular design: de novo design techniques; quantitative structure activity relationships (QSAR); comparative molecular field analysis (CoMFA); docking; molecular diversity and combinatorial libraries.

C581 Macromolecular Structure and Interaction (3 cr.) Principles of inter- and intra- molecular interactions; structural stability of proteins and nucleic acids; thermodynamic and kinetic analysis of complex binding; experimental methods for analysis of macromolecular structure and binding.

C582 Biomolecular Catalysis (3 cr.) P Theory and analysis of biochemical catalysis; enzyme kinetics; cofactors; regulation of enzymatic reactions.

C585 Structure and Function of Biological Membranes (3 cr.) Biochemistry and biophysics of lipids, membranes, and membrane proteins; fundamentals of membrane transport; interfacial catalysis; transmembrane signal transduction.

C611 Electroanalytical Chemistry (1.5-3 cr.) Theory and practice of electrochemical techniques (such as cyclic voltammetry, chronocoulometry, stripping analysis, thin-layer electrochemistry, and spectroelectrochemistry) used for analysis and for the characterization of inorganic and organic systems. (May be offered in alternate years.)

C612 Spectrochemical Methods of Analysis (1.5-3 cr.) New instrumentation and techniques employed in spectrochemistry; in-depth treatment of commonly used spectrochemical methods. (May be offered in alternate years.)

C613 Mass Spectrometry and Stable Isotopes (1.5-3 cr.) Topics in mass spectroscopic instrumentation and applications and in the natural chemistry of the stable isotopes of C, H, N, O, S, and rare gases. (May be offered in alternate years.)

C614 Chromatography (1.5-3 cr.) Theoretical and practical aspects of chromatographic methods of separation; fundamentals of gas and liquid chromatography, related instrumentation, and selected applications. (May be offered in alternate years.)

C615 Bioanalytical Chemistry (1.5-3 cr.) Survey of modern analytical techniques, including spectrochemical, electrochemical, and separation methods, used in biochemical analysis and their applications. (May be offered in alternate years.)

C616 Surface Analysis and Surface Chemistry (1.5 cr.) An overview of the modern instrumental techniques of surface analysis will be presented, together with a survey of their applications to solve surface chemical problems. Topics include electron and ion spectroscopies, SIMS, LEED, thermal desorption spectroscopy, surface electron and ion microscopies, catalysis, microelectronics fabrication, and corrosion.

C619 Seminar: Analytical Chemistry (1 cr.) P: consent of instructor. Individual student seminars covering new methods or applications of chemical analysis or characterization. Required of all analytical chemistry majors.

C630 Structure and Bonding (3 cr.) P: C502 and C561. Applications of quantum mechanics to the electronic and geometric structure of inorganic molecules. Advanced ligand field and molecular orbital theories. The Jahn-Teller effects and orbital symmetry studies of stereochemistry. Inorganic photochemistry. (May be offered in alternate years.)

C632 Structure, Function, and Spectroscopy of Metal Ions in Biological Systems (3 cr.) Introduction to the field of bioinorganic chemistry and spectroscopic methods for determining structure/function relationship of metal ions in biology. Emphasis on oxygen carriers, metal ion transport and storage, as well as oxidoreductases involved in oxygen, hydrogen, and nitrogen metabolism. A discussion of electron transfer proteins, photosystems, and the role of metals in medicine will also be included.

C633 Inorganic Chemistry of Main Group Elements (3 cr.) The syntheses, structure, and industrial application of compounds and materials in which main group elements play a major role. All elements except the d-block transition metals are included as main group elements. This includes the f-block lanthanides and actinides as well.

C634 Transition Metal Chemistry (3 cr.) Survey of the properties of the transition metals with emphasis on common oxidation levels, coordination geometries, and compounds with "classical" ligands; "hard" and "soft" acids and bases; d-orbitals and their energies in different geometries; formation constants and the Chelate Effect; the Jahn-Teller theorem; low-, intermediate-, and high-spin systems; mixed valency; metal-ligand multiple bonding, metal-metal bonds; coordination clusters and their biological relevance.

C635 Mechanisms of Inorganic Reactions (3 cr.) Analysis of the experimental and theoretical basis for our understanding of the reactions associated with main group and transition metal ions and inorganic reagents in solution. Classes of reactions include ligand substitutions, redox reactions, electron transfer reactions, reactions within the coordination sphere of metal ions including catalysis by photochemical and electrochemical activation.

C636 Organometallic Chemistry and Catalysis (3 cr.) Synthesis and reactivity of organo-main group and transition metal compounds, including application to organic synthesis. Predictive principles and generic C-C and C-H bond-forming reactions, including hydrogenation, coupling, addition to olefins or alkynes, and metatheses. These reactions are also extended to reactions on surfaces and solid-state processes.

C637 Physical Methods in Structural Chemistry (3 cr.) Application of X-ray diffraction, dynamic NMR and mass spectroscopy to structural and mechanistic problems throughout the periodic table, with emphasis on what techniques are optimal for particular questions, as well as the potential weaknesses of each.

C638 Seminar: Inorganic Chemistry (1-3 cr.) P: consent of instructor. Topics not ordinarily covered by regularly scheduled courses, such as boron hydrides, X-ray diffraction, metal-metal bonds, bioinorganic chemistry, platinum metals chemistry, inorganic photochemistry, etc. (May be offered in alternate years.)

C639 Characterization of Paramagnetic Molecules (3 cr.) Definitions of diamagnetism, paramagnetism, magnetization and magnetic susceptibility; the Curie Law; orbital angular momentum; the Van Vleck equation; zero-field splitting; exchange interactions in dinuclear and polynuclear metal clusters. Basic concepts of paramagnetic NMR; spin delocalization mechanisms and isotropic shifts; contact and dipolar contributions. EPR of transition complexes; g-value anisotropy as a function of coordination geometry.

C643 Organic Natural Products (3 cr.) P: C540 and C543; or consent of instructor. Synthesis and chemical-physical analysis of the structure of alkaloids, antibiotics, bacterial metabolites, plant pigments, steroids, and terpenes. (May be offered in alternate years.)

C644 Physical Organic Chemistry (1-3 cr.) P: C342 and C362. Application of physical-chemical techniques to the study of structure and mechanism of reaction of organic compounds.

C648 Seminar: Organic Chemistry (1-3 cr.) P: consent of instructor. Recent developments in such areas as sulfur compounds, heterocycles, stereochemistry, polymers, and synthesis. (May be repeated.)

C668 Seminar: Physical Chemistry (1-3 cr.) P: consent of instructor. Topics such as chemical applications of matrix algebra and group theory, digital computing techniques, solid state chemistry, high temperature processes, electrochemistry, theory of solutions, spectroscopy, and surface chemistry. (May be repeated.)

C681 Advanced Protein Biosynthesis and Processing (1.5 cr.) Detailed analysis of protein synthesis, post-translational modification, and macromolecular assembly, including the role these modifications play in mature protein function, biosynthesis, structure, function, and analysis of complex oligosaccharides.

C683 Advanced Nucleic Acid Biochemistry (1.5 cr.) Mechanistic analysis of nucleic acid metabolism; specificity and role of DNA polymerases and repair pathways; DNA replication and recombination mechanisms; RNA structural motifs and physical properties; RNA synthesis and processing in gene expression; catalytic RNA molecules; applications of RNA molecules.

C685 Advanced Macromolecular Structure and Interaction (1.5 cr.) Supplements and extends B503; emphasis on stability and folding mechanisms of proteins and nucleic acids and detailed thermodynamic analysis of binding interactions.

C686 Structural Methods (1.5 cr.) Fundamental principles of circular dichroism, nuclear magnetic resonance, and X-ray crystallography in the study of protein and nucleic acid structures. Theoretical and practical aspects will be presented, with particular emphasis on application strategies.

C687 Seminar: Advanced Topics in Biochemistry (1-3 cr.) P: Consent of Instructor. Topics vary yearly and include the following: physio-chemical techniques in the study of macromolecules; experimental methods in enzymology; organic chemistry of enzymatic reactions and enzyme models; conformational properties and macromolecules. Credit given for only one of the following C687, B680.

C688 Seminar in Biochemistry Attendance and participation in the weekly Biochemistry Program seminar series.

A800 Seminar: Analytical Chemistry (1 cr.)

B800 Seminar: Biological Chemistry (1 cr.)

N800 Seminar: Inorganic Chemistry (1 cr.)

P800 Seminar: Physical Chemistry (1 cr.)

R800 Seminar: Organic Chemistry (1 cr.)

C810 Research: Analytical Chemistry (cr. arr.)**

C830 Research: Inorganic Chemistry (cr. arr.)**

C840 Research: Organic Chemistry (cr. arr.)**

C860 Research: Physical Chemistry (cr. arr.)**

C880 Research: Biological Chemistry (cr. arr.)**

**These courses are eligible for a deferred grade.