The Ottawa-Carleton Chemistry Institute

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The Institute

Director of the Institute:
A.G. Fallis
Associate Director of the Institute:
G.W. Buchanan

The Ottawa-Carleton Chemistry Institute, established in 1981, is a joint program of graduate studies and research in chemistry for Carleton University and the University of Ottawa. The Institute combines the research strengths and resources of the Departments of Chemistry at both campuses. Research facilities are shared and include: a major mass spectrometry centre, X-ray spectrometer, several modern NMR spectrometers, a pico-second laser facility, an ultratrace analysis laboratory, and an electrochemical research centre. In addition, the resources of many federal departments are available to graduate students, including the National Research Council and its library, the National Science Library (CISTI), and departments of Health and Welfare and Agriculture.

The Institute offers the M.Sc. and Ph.D. degrees in all areas of chemistry, including biochemistry, analytical, inorganic, organic, physical and theoretical chemistry. All thesis, seminar and examination requirements may be met in either English or French. Students will be enrolled at the campus where the research supervisor is located. Several graduate students also conduct their research off campus under the supervision of one of the Institute's adjunct professors.

Application forms and further information may be obtained by writing to the director of the Institute.

Ottawa-Carleton Collaborative Program in Chemical and Environmental Toxicology

The Departments of Chemistry and Biology at Carleton University and the University of Ottawa, and the Department of Psychology at Carleton University, provide a collaborative program in chemical and environmental toxicology at the M.Sc. level. For further details, see page 166.

Members of the Institute

Howard Alper, *Organometallic Chemistry*
J.W. ApSimon, *Natural Products Chemistry*
M.H. Back, *Chemical Kinetics and Photochemistry*
H.H. Baer, *Carbohydrate Chemistry*
R.G. Barradas, *Electrochemistry*
A.D.O. Bawagan, *Chemical Physics*
D.M. Bishop, *Theoretical Chemistry*
G.W. Buchanan, *Applications of NMR Spectroscopy*
P.H. Buist, *Bio-organic Chemistry*
C.L. Chakrabarti, *Analytical Chemistry, Environmental Chemistry*
B.E. Conway, *Electrochemistry*
R.J. Crutchley, *Physical Inorganic Chemistry*
Christian Detellier, *Bio-inorganic Chemistry*
Tony Durst, *Synthetic and Medicinal Organic Chemistry*
A.G. Fallis, *Synthetic Organic Chemistry*
R.R. Fraser, *Physical Organic Chemistry*
Sandro Gambarotta, *Inorganic Chemistry*
I. Hamilton, *Theoretical Chemistry*
B.R. Hollebone, *Chemical Spectroscopy and Chemical Toxicology*
J.L. Holmes, *Mass Spectroscopy*
K.U. Ingold, *Physical Organic Chemistry, Free Radicals*
Harvey Kaplan, *Biochemistry*
J.A. Koningstein, *Chemical Physics*
Peeter Kruus, *Solution Physical Chemistry, Ultrasonics*
E.P.C. Lai, *Photoacoustic Spectroscopy, Analytical Chemistry*
K.J. Laidler, *Reaction Kinetics*, Professor Emeritus
B.A. Morrow, *Surface Chemistry and Catalysis*
D.S. Richeson, *Inorganic, Solid State and Organometallic Chemistry*
J.A. Ripmeester,* *Colloid and Clathrate Chemistry*
René Roy, *Organic Chemistry*
J.C. Scaiano, *Photochemistry*
I.C.P. Smith,* *NMR Studies of Biologically Important Molecules*
K.B. Storey, *Enzyme Biochemistry, Biotechnology*
Heshel Teitelbaum, *Chemical Kinetics*
C.S. Tsai, *Enzyme Action and Yeast Cultures*
Z.Y. Wang, *Synthetic Polymer Chemistry and Organic Chemistry*
D.C. Wigfield, *Organic Reaction Mechanisms, Mechanisms in Toxicology*
C.P. Wilde, *Electrochemistry*
J.S. Wright, *Theoretical Chemistry*

* Adjunct Research Professor

Master of Science

Admission Requirements

The normal requirement for admission to the program is an honours B.Sc. degree in Chemistry, with a B+ average in the last two years and a B average overall. Applicants who do not meet this requirement, or whose undergraduate degree is in another, closely related field, may be accepted into the program, but may be assigned extra courses.

Program Requirements

- A research thesis, which must be defended at an oral examination
- Two graduate courses (one semester each)
- One seminar course (two semesters)

Doctor of Philosophy

Admission Requirements

The normal requirement for admission to the Ph.D. program is a B.Sc. or an M.Sc. degree in Chemistry.

Program Requirements (from B.Sc.)

- A research thesis, to be defended before an examination board which will include an external examiner
- A comprehensive examination in chemistry; the format of this examination depends on the field of chemistry in which the student is conducting his/her research. At Carleton this normally takes the form of a research proposal
- Four graduate courses (one semester each)
- Two seminar courses (two semesters each)

Program Requirements (from M.Sc.)

As above, except that credit for up to two graduate courses may be given to reduce the requirement for graduate courses from four to two.

Residence Requirements

For the M.Sc. degree:

- at least one year of full-time study

For the Ph.D. degree (from B.Sc.):

- at least three years of full-time study

For the Ph.D. degree (from M.Sc.):

- at least two years of full-time study

Graduate Courses*

- Chemistry 65.509 (CHM8150)

Special Topics in Molecular Spectroscopy
Topics of current interest in molecular spectroscopy. In past years, the following areas have been covered: electronic spectra of diatomic and triatomic molecules and their interpretation using molecular orbital diagrams; Raman and resonance Raman spectroscopy; symmetry aspects of vibrational and electronic levels of ions and molecules in solids the presence of weak and strong resonant laser radiation.
(Also offered as Physics 75.522/PHY8122)

- Chemistry 65.511(CHM8181)

Chemical Physics of Electron-Molecule Collisions
Basic classical scattering theory and quantum mechanical scattering theory. Experimental aspects, such as electron optics, electron gun fundamentals, energy analyzers and electron detectors. Applications to the understanding of the chemistry of materials.

- Chemistry 65.516 (CHM8170)

Quantum Chemistry
Molecular orbital theory and its application to chemistry. Self-consistent field method, results for diatomic molecules. Configuration interaction and molecular dissociation. Basis sets and molecular properties. *Ab initio* versus semi-empirical approaches. Correlation diagrams for chemical reactions. Poly-atomic molecules and potential energy surfaces.

- Chemistry 65.517 (CHM8161)

Physical Chemistry of Solutions
Major theoretical approaches and experimental methods used in the study of liquids and solutions. *Prerequisite:* A reasonable background knowledge in thermodynamics, quantum chemistry and statistical mechanics.

- Chemistry 65.519 (CHM8149)

Molecular Reaction Dynamics
State-to-state versus bulk reaction kinetics. Trajectory approach to molecular reaction dynamics. Important experimental techniques: molecular beam reactions infrared chemi-luminescence, laser-induced fluorescence, chemical lasers. Use of trajectory calculations to interpret experiments and to provide reaction mechanisms.

- Chemistry 65.520 (CHM8152)

Surface Chemistry and Catalysis
Adsorption phenomena and isotherms, surface area of solids. Modern techniques in surface chemistry and surface science such as electron diffraction, Auger electron spectroscopy, photo-electron spectroscopy, electron energy loss spectroscopy, infrared and Raman spectroscopy. Current new techniques.

- Chemistry 65.522 (CHM 8131)

Physical Chemistr

* F,W,S indicates term of offering. Courses offered in the fall *and* winter will be followed by T.
The number following the letter indicates the credit weight of the course: 1 denotes a half-course credit, 2 denotes a full-course credit, etc.

y of Electrolytic Solutions
Properties of water, hydration of ions, ionic interaction, colloidal and polymeric electrolytes. Ionization processes in solution.

- Chemistry 65.523 (CHM8141)

Applied Electrochemistry
Selected topics in applied electrochemistry will be reviewed including metal electrodeposition, organic electrochemistry, performance of batteries, electrochemical energy conversion, corrosion and passivity. Electrochemistry at semiconductors.

- Chemistry 65.524 (CHM8151)

Electrochemistry at Interfaces
Introduction to electrode processes and electrolysis. Potential differences at interfaces. Characterization of the electrical double layer. Dipole orientation effects; charge transfer in absorbed layers; electrochemical origins of surface science concepts. Theory of electro transfer; electrode kinetics; electrocatalysis. Industrial applications; photo-electrochemistry.

- Chemistry 65.525 (CHM8129)

Chemistry of Natural Products
Synthesis of natural products. Strategies for development of a synthetic method. Preservation and development of chiral centres. Examples of synthesis are taken from the current literature; students will be asked to develop syntheses for various target molecules.

- Chemistry 65.527 (CHM8121)

Organic Reaction Mechanisms
Advanced physical organic chemistry, including topics such as: acidity functions, pK_a's of organic compounds, steric and electronic effects in organic chemistry, molecular orbital theory and correlation diagrams, structure calculations using molecular mechanics.

- Chemistry 65.528 (CHM8133)

Multinuclear Magnetic Resonance Spectroscopy
Principles of Nuclear Magnetic Resonance (NMR). The NMR parameters to be studied are: chemical shift, spin-spin coupling, electric quadrupole coupling, spin-spin and spin-lattice relaxation rates. NMR and the periodic table. Dynamic NMR. Applications in chemistry and biochemistry. The Fourier Transform technique. Pulse sequences. Basic principles and applications of two-dimensional NMR.

- Chemistry 65.529 (CHM8154)

Reaction Intermediates
Introduction to the basic principles of photo-chemistry in condensed phases as a method for the generation of reactive intermediates. This is followed by a series of selected topics to cover various types of reaction intermediates and the techniques for their study. Topics include: excited states, free radicals, carbenes, biradicals, enols, carbocations and zwitterionic intermediates. The techniques include laser and conventional flash photolysis, pulse radiolysis, esr, CIDNP and matrix isolation. Several of these topics are covered in student seminars.

- Chemistry 65.530 (CHM8159)

Total Synthesis: Strategies and Case Studies
General procedures for the total synthesis of natural products will be examined. A general discussion of retrosynthetic planning, choice of starting materials, multiple bond construction, stereochemical considerations and choice of strategies will be followed by the analysis of recent syntheses. Comparison of alternative solutions emanating from different laboratories will be studied as will recent trends including pericyclic reactions, free radical cyclizations, etc. A reasonable knowledge of modern organic reactions is assumed.

- Chemistry 65.531 (CHM8160)

Chiron Approach to Natural Product Syntheses
Retrosynthetic analysis and description of natural product total synthesis through the chiron strategy with emphasis on carbohydrates and amino acids as chiral building blocks. Macrolides and polyether synthesis. Diversity in carbohydrates; chiral templates and their selective manipulations. Aspects of protecting group chemistry, stereoelectronic effects, and chirality induction and transfer.

- Chemistry 65.532 (CHM8132)

Enzymology and Protein Chemistry
Basic principles of structure-function relationships in proteins. Chemical nature of polypeptides and the folded conformation of proteins. Enzymatic catalysis; protein engineering.

- Chemistry 65.533 (CHM8126)

Bioorganic Chemistry
Overview of recent developments in the general area of biocatalysis. Current examples of the biotransformation of organic compounds using enzyme models, abzymes, enzymes, immobilized enzymes, microbial cells and recombinant microbial cells. Biosynthetic procedures of industrial importance in waste management.

- Chemistry 65.539 (CHM8144)

Electron Transfer Reactions: Theory and Experiment
Bimolecular electron transfer theory as developed by Marcus in the 1950s. Experimental verification of Marcus theory. Recent advances in long-range intramolecular electron transfer. Particular emphasis will be given to the mechanism of electronic coupling between donor and acceptor.

- Chemistry 65.540 (CHM8114)

Special Topics in Non-Metal Chemistry
Topics of current interest in non-metal chemistry. The content of this course may vary from year to year.

- Chemistry 65.541 (CHM8117)

Organometallic Chemistry
A discussion of the formation, character, bonding and reactions of compounds containing organic ligands bound to metals through from one to eight carbon atoms. Industrial processes (olefin meta-thesis, the OXO process, the Monsanto acetic process, etc.) and biological processes (e.g. reactions catalyzed by coenzyme B_{12}) are also examined. The emphasis is on transition metal chemistry, including synthesis and mechanisms of the reactions concerned, and on the physical techniques available for characterization of the compounds.

- Chemistry 65.542 (CHM8115)

Special Topics in Inorganic Chemistry
Topics of current interest in inorganic chemistry. In the past, the course has covered Ceramics: binary and ternary phase diagrams and their thermodynamic basis; pyrometallurgical and ceramic thermochemistry; glasses; molten salts and solid solutions; defects; doping and preparation of pure materials; electrical and surface properties of ceramics.

- Chemistry 65.543 (CHM8112)

Methods in Analytical Chemistry
The critical evaluation and selection of analytical techniques. Areas to be covered include: analytical aspects of atomic spectroscopy, electro-chemistry, chromatography, molecular spectrometry, mass spectrometry. This course provides a sound basis for choosing the best analytical technique for a particular problem. The focus will be on: when a technique is applicable; limitations, advantages and disadvantages; detection limits, sensitivity and interference; commercially available instrumentation.

- Chemistry 65.544 (CHM8125)

Organic Synthesis (Carbanion Chemistry)
Discussion of recent developments in the use of carbanion chemistry for the making of carbon-carbon and carbon-heteroatom bonds. Particular emphasis is given to methods which yield optically active products. In the most recent course the following topics were covered: methods of generating carbanions, kinetic versus thermo-dynamic acidity, hetero-atom-stabilized carbanions, the aldol and related condensations, Michael addition reactions, and ortho-metalation in aromatic systems.

- Chemistry 65.545 (CHM8127)

Chemistr
y of
Carbohyd
rates
Nomenclature. Chemistry and synthesis carbohydrates. Chemical modifications. Chemistry and synthesis of flavinoids and carotenoids.

- Chemistry 65.546 (CHM8164)

Organic Polymer Chemistry
Introduction to basic principles of polymer chemistry, industrial and synthetic polymers, different types of polymerization and polymer characterization. This is followed by a series of selected topics to cover some important polymers with emphasis on the synthesis, such as commodity plastics, engineering thermoplastics and specialty polymers.
Prerequisites: Chemistry 65.321 and 65.322 and/or 65.423 or equivalent. Students should have a basic knowledge of organic reaction mechanisms and stereochemistry.

- Chemistry 65.547 (CHM8134)

Spectroscopy for Organic Chemists
Analysis of proton NMR spectra. Fourier transform ^{13}C NMR, strategies for structure elucidation relaxation times, two-dimensional NMR. Aspects of mass spectrometry.

- Chemistry 65.548 (CHM8122)

Special Topics in Organic Chemistry
Topics of current interest in organic chemistry. In the past one course has covered solid state NMR: chemical aspects of solid state structure; molecular ordering and motion in the solid state; magnetic interactions; hydrogen, deuterium and ^{13}C NMR; experimental methods; applications; relationship between high resolution solid-state and solution NMR.

- Chemistry 65.549 (CHM8123)

Recent Advances in Organic Chemistry
Topics of current interest will be discussed.

- Chemistry 65.550 (CHM8116)

Analytical Instrumentation
Principles of modern electronic instrumentation and their application in the chemical laboratory. Scientific instruments; measurement and control systems; microcomputer interfacing. Instrumentation concepts including feedback control, signal-to-noise enhance-ment, data acquisition, and signal processing will be presented along with the techniques and devices for their implementation. A parallel laboratory is taught using modern test instruments. Examples include absorption spectrophotometer, derivative titration thermocouple, pH meter, and cyclic voltammetry.

- Chemistry 65.551 (CHM8220)

Problems in Organic Chemistry
The
pro
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lems which are assigned in this course are of two types: (1) written examinations on a particular topic in organic chemistry, (2) critical reviews of papers in the current organic literature, i.e. a simulated referee's report on the paper. In order to pass the course, eight "problems" must be solved satisfactorily.

- Chemistry 65.552 (CHM8110)

Analytical Approach to Chemical Problems
Case-study approach to a variety of problems in agricultural, biochemical, environmental, food processing, geological, industrial and surface sciences that can be solved by analytical chemistry. Comparative study of analytical methods appropriate to each case includes: capillary electrophoresis, chemiluminescence, electrochemical biosensors, Fourier transform infrared spectroscopy, inductively coupled plasma emission, neutron activation analysis, sensor arrays, secondary ion mass spectrometry, tandem mass spectrometry, and ultra-high resolution nuclear magnetic resonance spectroscopy. Modern data analysis techniques such as pattern recognition are also discussed.

- Chemistry 65.553 (CHM8108)

Analytical Mass Spectrometry
The course consists of four sections. 1) The basics of mass spectrometry and gas phase ion chemistry. 2) The instrumentation currently available and the principles of its operation. Methods of ionization. 3) separation techniques, their successes and limitations when connected to a mass spectrometer. 4) The obtaining and interpretation of data. The relationships between mass spectra and chemical structure.

- Chemistry 65.555 (CHM8119)

Advanced Ultratrace Analytical Chemistry
Criteria for evaluation and selection of analytical techniques and methods. Simultaneous and sequential multielement analysis. Atomic absorption, atomic emission and atomic fluorescence spectrometry, using optical spectrometric and mass-spectrometric determination. Electroanalytical techniques. Applications of these techniques at trace and ultra-trace levels in complex matrices.

- Chemistry 65.556 (CHM8120)

Environmental Analytical Chemistry of Inorganic Systems
Sampling of the atmospheric and the aquatic environment. The problems of sampling artifacts and of blanks in the sub-parts-per trillion concentration levels. Analytical techniques and methods for quantitative determination of analytes in elemental and isotopic form. Analytes in molecular form and analytical techniques for chemical speciation. Advantages and limitations of various speciation schemes.

- Chemistry 65.557 (CHM8162)

Environmental Organic Chemistry
Methods for determination of organic analytes in environmental systems. All aspects of a method will be discussed, including sampling, sample treatment, measurement, quality control, and data significance. Application to such environmentally important analytes as PCG's, dioxins, pesticides, herbicides, trihalomethanes, and polycyclic aromatic hydrocarbons. Rationale and selection of specific methods.

- Chemistry 65.558 (CHM8163)

Special Topics in Analytical Chemistry
Topics of current interest in analytical chemistry. The content of this course may change from year to year.

- Chemistry 65.561 (CHM8118)

Advanced Physical Inorganic Chemistry
Application of quantum theory to inorganic spectroscopy and magnetism. Use of quantum mechanics and group theory to identify states and processes in inorganic spectroscopy. The basic theory is applied to structure analysis and prediction of reactions, and provides a model for inorganic photochemistry.
Prerequisite: A reasonable background in quantum mechanics and group theory.

- Chemistry 65.570 (CHM8143)

Special Topics in Physical Chemistry
Topics of current interest in physical chemistry. The content of this course may change from year to year.

- Chemistry 65.571 (CHM8145)

Photochemistry
Photochemical reactions of small molecules and the relation to atmospheric chemistry. Lasers and applications to measurements of the dynamics of elementary reactions. Production and detection of reactive species. Energy transfer processes. Photolysis of formaldehyde and carbonyl compounds. Multiphoton absorption of infrared radiation.

- Chemistry 65.572 (CHM8135)

Theories of Chemical Reaction Rates
Concepts and theories of chemical kinetics. Significance of activation energy; transition state theory and more modern developments; reaction dynamics. Other optional topics include unimolecular gas reactions, theory of solvent effects, homogeneous and heterogeneous catalysis, and kinetic isotope effects.

- Chemistry 65.573 (CHM8137)

Advanced Chemical Kinetics
Study of the principles involving the exchange of translational, rotational, vibrational and electronic energy in molecular collisions. Influence of energy transfer processes on thermal unimolecular and biomolecular reactions. Study of the relationship between microscopic and macroscopic kinetics of elementary reactions.

- Chemistry 65.574 (CHM8142)

Symmetry in Chemistry
Introduction to group theory with emphasis upon irreducible representations. Application to molecular vibrations, molecular orbital theory and transition metal chemistry.

- Chemistry 65.575 (CHM8140)

Chemical Spectroscopy
Interaction of radiation with matter. Additional topics, which will depend on the nature of the class, will be chosen from the following: perturbation methods for studying atomic spectra, fundamentals of ESR and NMR spectroscopies; rotational and vibrational spectra of diatomic and polyatomic molecules, group theory as applied to molecular vibrations.
Prerequisite: A background in quantum mechanics at the undergraduate level.

- Chemistry 65.576 (CHM8148)

Gas Phase Ion Chemistry
Structure, energetics and reaction kinetics of ions in the gas phase. Small organic ions, chemistry of free radicals, hypervalent species. Contemporary experimental methods in the physical chemistry of fast ion beams. Emphasis will also be upon recent work on novel ions and neutral species of relevance to interstellar chemistry.

- Chemistry 65.577 (CHM8138)

Enzyme Kinetics and Mechanism
Kinetic studies of enzymic reactions. Enzyme efficiency, specificity and versatility. Mechanisms and regulation of enzymic reactions. Analyses of enzymic systems.

- Chemistry 65.578 (CHM8156)

Principles of Toxicology
The basic theorems of toxicology with examples of current research problems. The concepts of exposure, hazard and risk assessment will be defined and illustrated with experimental material from some of the more dynamic areas of modern research.
(Also offered as Biology 61.642 and Psychology 49.525)

- Chemistry 65.579 (CHM8157)

Chemical Toxicology
An advanced course in chemical toxicology which deals with both chemical hazard and exposure. An overview of the empirical data relating to the toxicity of various classes of chemicals to test organisms is followed by a treatment of toxicity at the cellular level, including studies of interaction between toxic substances and enzymatic systems. This is the type of data which a student could apply to the interpretation and monitoring of the new WHMIS health regulations. Initial events in enzyme induction and mutagenesis are considered. Predictive capabilities in the areas of structure-activity relationships and mechanisms of enzyme induction are considered, followed by an assessment of mechanism of exposure of toxic chemicals.

- Chemistry 65.581 (CHM8256S)

Seminar I

- Chemistry 65.582 (CHM8257S)

Seminar II

- Chemistry 65.585 (CHM8167)

Seminar in Toxicology
A two-term course in seminar format, highlighting current topics in toxicology. The course will feature student, faculty and invited seminar speakers.
(Also offered as Biology 61.645 and Psychology 49.526)

- Chemistry 65.590 (CHM8158)

Directed Special Studies
Under unusual circumstances and with the recommendation of the research supervisor, it is possible to engage in directed study on a topic of particular value to the student. This may also be used for credit if there are insufficient course offerings in a particular field of chemistry.

- Chemistry 65.599 (CHM7999)

M.Sc. Thesis

- Chemistry 65.699 (CHM9999)

Ph.D. Thesis