

## The Ottawa-Carleton Chemistry Institute

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### The Institute

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*Director of the Institute:*

G.W. Buchanan

*Associate Director of the Institute:*

René Roy

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 173.

### Members of the Institute

Howard Alper, *Organometallic Chemistry*  
J.W. ApSimon, *Natural Products Chemistry*  
M.H. Back, *Chemical Kinetics and Photochemistry*  
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*  
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  
J.B. Milne, *Chemistry of Non-Metals*  
Mario Morin, *Interfacial Chemistry*  
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*  
A.St.-Amant, *Theoretical and Computational Chemistry*  
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*

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\* Adjunct Professor, Adjunct Research Professor

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## Master of Science

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### 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)
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## Doctor of Philosophy

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### 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

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## Graduate Courses\*

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- 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. Polyatomic 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 65.520 (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.

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\* 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.

- Chemistry 65.522 (CHM8131)

Physical Chemistry 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 adsorbed layers; electrochemical origins of surface science concepts. Theory of electron transfer; electrode kinetics; electrocatalysis. Industrial applications; photo-electrochemistry.

- 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 65.538 (CHM8122)

Solid State Chemistry

Thermodynamic and kinetic aspects of solid state synthesis. Spectroscopic and structural characterization of solids. Chemical and physical properties of solids including intercalation reactions, ionic conductors, glasses, electronic, magnetic, optical, and physical/mechanical properties.

Before 1994-95 course 65.538 (CHM8122) was offered as 65.545 (CHM8127).

- Chemistry 65.539 (CHM8144)

Electron Transfer Reactions: Theory and Experiment

Development of electron transfer theory from classical, semi-classical to quantum mechanical treatments. Recent experimental results related to classical

Marcus electron transfer theory and the application of electron transfer theory to biological processes.

- 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 metathesis, the OXO process, the Monsanto acetic process, etc.) and biological processes (e.g. reactions catalyzed by coenzyme B<sub>12</sub>) 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 thermodynamic acidity, heteroatom-stabilized carbanions, the aldol and related condensations, Michael addition reactions, and ortho-metalation in aromatic systems.

- 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.

Also offered at the undergraduate level, with different requirements, as 65.424, for which additional credit is precluded.

- Chemistry 65.547 (CHM8134)

Spectroscopy for Organic Chemists

Analysis of proton NMR spectra. Fourier transform <sup>13</sup>C NMR, strategies for structure elucidation relaxation times, two-dimensional NMR. Aspects of mass spectrometry.

Also offered at the undergraduate level, with different requirements, as 65.442, for which additional credit is precluded.

- 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 <sup>13</sup>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 enhancement, 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 problems 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 ultratrace levels in complex matrices.

- 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 65.570 (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 65.576 (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 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