

# CHEMISTRY

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## Courses

All courses are six week modules and are equivalent to one half of a term course (1.5 credit units in weight) with the exception of CHEM 801, CHEM 802, CHEM 803, CHEM 905, CHEM 910 (all 3.0 credit units) and CHEM 899 and CHEM 999 (6.0 credit units).

Students should review the department's website for the most current list of courses available and terms offered.

### **CHEM 801 Safety in the Laboratory**

An introduction to safety procedures and the safe handling of chemical compounds and equipment in the laboratory. This non-credit course is offered every year to students from other departments. Fall. P. Jessop (Coordinator)

### **CHEM 802 Chemistry Seminar Program**

Based on the regular departmental seminar program offered during the fall, winter and summer, this non-credit course is to be taken every year by all graduate students. As part of this course M.Sc. and Ph.D. students must attend a minimum number of departmental seminars. In addition, Ph.D. students will present one seminar on their research prior to their thesis submission. Fall/Winter/Summer. G. Howe (Seminar Coordinator). Website: Departmental Seminar Series (<https://www.chem.queensu.ca/departmental-seminar-series/>).

### **CHEM 803 Principles of Scientific Communication**

Principles of scientific verbal and written communication in Chemistry. Topics include computer literature searching, scientific writing techniques (for research reports, journal manuscripts, and theses), oral and poster conference presentations, and communication skills as teaching assistantships. Assignments will include completion of online course modules on scientific communication from MyGradSkills.ca. Fall. A. Bongers.

### **CHEM 805 NMR Methods for Structure Identification**

An introductory course on identification of organic and organometallic compounds using multinuclear NMR techniques. The focus will be on practical applications for those working in synthetic chemistry. Winter. F. Sauriol.

### **CHEM 806 Multidimensional NMR techniques**

Advanced methods for the identification of organic and organometallic compounds using multinuclear NMR techniques. The focus will be on practical applications for those working in synthetic chemistry. Winter. F. Sauriol. PREREQUISITE: CHEM 805.

### **CHEM 810 Materials Characterisation Methods**

A survey of materials characterisation methods with an emphasis on practical applications in materials and polymer chemistry. Techniques will include electron microscopy, scanning probe methods, photoelectron & Auger spectroscopy, cyclic voltammetry and powder X-ray diffraction methods. Not offered in 2022-2023.

### **CHEM 814 Carbohydrate Chemistry**

An introduction to the chemistry of carbohydrates: Monosaccharides and their derivatives; Strategies for making glycosidic bonds and synthesizing oligosaccharides; Chemical and biochemical aspects of complex oligosaccharides and glycoconjugates. (1.5 credit units). Not offered in 2022-2023.

### **CHEM 817 Industrial Synthesis of Fine Chemicals**

Industrial processes for the synthesis of vitamins, pharmaceuticals and related fine chemicals represent practical solutions to complex problems in chemical synthesis; selected case studies will be examined. Not offered in 2022-2023.

### **CHEM 819 Current Topics in Physical and Theoretical Chemistry**

A critical review of the current research literature with strong emphasis on student discussions and presentations. Topics are selected from recent examples in the literature and may include light-matter interactions, nanostructures, surface probe studies, computational methods and other examples in physical chemistry and molecular physics. Winter. P. Duchesne.

### **CHEM 820 Magnetic Resonance**

This course will cover subject areas of magnetic resonance spectroscopy including nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), nuclear quadrupole resonance (NQR) and magnetic resonance imaging (MRI). Fall. G. Wu.

### **CHEM 834 Molecular Orbitals and Structures**

An overview of modern computational techniques and software for the determination of molecular orbitals and structures. Intended as a general introduction for graduate students of all disciplines. Offered jointly with CHEM 413. Fall. F. Heidar-Zadeh.

EXCLUSION: CHEM 413

### **CHEM 838 Numerical Methods in Chemistry**

Topics include numerical integration, numerical treatment of differential equations, interpolation, Fourier transforms, regression. Concepts in Fortran programming are also introduced. Not offered in 2022-2023.



#### **CHEM 840 Modern Mass Spectrometry**

An introduction to modern mass spectrometry. Instruments and the various methods of forming or introducing ions into the gas phase will be discussed and mass spectra will be interpreted. Offered jointly with CHEM 411. Fall. D. Beauchemin.

EXCLUSION: CHEM 411

#### **CHEM 842 Applications of Modern Mass Spectrometry**

This module focuses after a brief review of ionisation techniques and current mass spectrometric equipment on novel hybrid-tandem-MS instruments and current applications of mass spectrometry in different areas of the life sciences. Topics include, but are not limited to, atomic composition determination, identification methods for proteins and determination of post-translational modifications such as phosphorylation or glycosylation now widely used in the evolving field of proteomics, studies of non-covalent biomolecule interactions and new high-throughput screening techniques as employed in drug or catalyst development. Not offered in 2022-2023.

#### **CHEM 850 Polymer Physical Chemistry**

Specific properties of polymers (glass transition, crystallinity, poly-dispersity, etc.) and their dependence on macromolecular structure and isomerism. Fall. G. Liu.

#### **CHEM 853 Polymer Synthesis**

Polymer synthesis overview: step and chain polymerization (free-radical, ionic and insertion mechanisms) and reactions on polymers. Examples of polymers and their uses. Not offered in 2022-2023.

#### **CHEM 854 Polymer Characterization in Solution**

Dilute polymer solutions and phase separation behaviour. Polymer characterization including vapour pressure lowering, ebulliometry, osmometry, viscometry, gel permeation chromatography, light scattering and ultracentrifuge methods. Not offered in 2022-2023.

#### **CHEM 855 Polymer Characterization in the Solid State**

An overview of various methods to characterize polymers in the solid state, including thermal analysis, spectroscopy (infrared, ultraviolet-visible, and nuclear magnetic resonance), microscopy, and mechanical analysis. Not offered in 2022-2023.

PREREQUISITE: CHEM 850 or permission of the instructor.

#### **CHEM 857 Engineering Properties of Polymers**

Relationships between macromolecular structure, the physical properties of polymeric materials, and applications. Topics include conformation and configuration, the glass transition, rubber elasticity, flammability, viscoelasticity,

yielding, and fracture. Case studies in material selection will be included. Fall. S. Hesp.

#### **CHEM 860 Symmetry and Structural Determination by X-ray Crystallography I**

X-ray diffraction theory, crystal symmetry and International Tables in space groups. Not offered in 2022-2023.

#### **CHEM 861 Symmetry and Structural Determination by X-ray Crystallography II**

The practical aspects of x-ray diffraction analysis, including data collection, structural solution and refinement. Not offered in 2022-2023.

PREREQUISITE: CHEM 860.

#### **CHEM 863 Transition metal catalysis for organic synthesis**

A review of the basic reactions involving transition metal catalysts in transformations of organic compounds. Fundamental reactions such as oxidative addition, reductive elimination, migratory insertions and transmetalations will be covered. Different types of ligands and their bonding properties will also be covered. Reactions of importance to organic chemistry including hydrogenations, oxidations, cross coupling reactions, metathesis and other pertinent reactions will be covered. Offered jointly with CHEM 414. Fall. P.A. Evans.

EXCLUSION: CHEM 414

#### **CHEM 866 Supramolecular Chemistry**

A study of the intramolecular forces responsible for molecular recognition and host/guest interactions in organic and inorganic supramolecular complexes, including rotaxanes and catenanes. Synthesis, characterization, and applications of supramolecular complexes in catalysis, biomimicry, and nanotechnology. Fall. A. Petitjean.

#### **CHEM 867 Bioinorganic Chemistry**

Kinetics and mechanisms of reactions of transition metals in biological systems, including metalloproteins and metalloenzymes. Roles of metals in hydrolytic and redox enzymes, oxygen transport, development of model systems. Not offered in 2022-2023.

#### **CHEM 869 Topics in Inorganic/Organometallic Chemistry**

Topics to be covered in this course include (a) luminescent/electroluminescent compounds, (b) fullerene chemistry and (c) magnetic and electronic materials. Offered jointly with CHEM 423. Winter. L. Lee.

EXCLUSION: CHEM 423

#### **CHEM 873 Optical Spectroscopic Instruments for Chemical Analysis**

An examination of advanced methods of analysis using optical spectroscopic methods, with an emphasis on instrument components, such as laser light sources, charge-coupled and other solid state detectors, fibre-optics and optical waveguide technologies. Examples will be selected from ultraviolet-visible and infrared absorbance and luminescence measurements, spectroscopic imaging, cavity and loop ringdown spectroscopy, graphite furnace atomic absorption and ICP optical emission spectroscopy. Not offered in 2022-2023.

#### **CHEM 879 Chemical Separations**

This course is an introduction into the use of chromatographic and electrophoretic separation methods for chemical analysis. The goal of this course is to familiarize students with chromatographic and electrophoretic theory and develop a practical understanding of various chemical separation methods. Topics to be covered in detail are gas chromatography, liquid chromatography (reverse phase, hydrophilic interaction, normal phase and ion exchange), capillary electrophoresis (capillary zone electrophoresis, electrochromatography and micellar electrokinetic chromatography) as well as others. Not offered in 2022-2023.

#### **CHEM 880 Modern Synthetic Methods**

A discussion of some modern methods used in organic synthesis with an emphasis on stereoselective reactions; illustrations of the value and scope of the methods and applications in the synthesis of complex molecules. Not offered in 2022-2023.

#### **CHEM 882 Mechanistic Organic Chemistry**

Physical basis for organic chemistry, dealing with specific mechanistic pathways and the tools necessary for the understanding of organic reaction mechanisms. Not offered in 2022-2023.

#### **CHEM 883 Bioorganic Chemistry**

Enzyme mechanisms and inhibition, catalytic antibodies, stereochemical and other biological probes. Phosphoryl group transfer reactions. Winter. G. Howe.

#### **CHEM 891 Topics in Chirality**

A review of topics in chirality research to be given by a changing group of experts in the field. Topics may include: Chirality transfer; Chiral catalysis; Chiral materials; Chiral photonics; and Chiral separations. Not offered in 2022-2023.

#### **CHEM 892 Scientific Ethics**

A survey of the principles of scientific ethics, particularly for those who plan to supervise and conduct research in an academic or industrial setting. Topics will include an introduction to morals and ethical theory, the concept and development of professions, and ethical problem solving.

The course will include a series of case studies. Not offered in 2022-2023.

#### **CHEM 893 Experimental Design**

The statistical design of experiments and the analysis of data in chemical synthesis and chemical process investigations are considered. Empirical modelling of process behaviour is studied. Applications of factorial and fractional factorial experimental designs in screening studies and methods of response surface exploration are examined. Not offered in 2022-2023.

EXCLUSION: CHEE 801

#### **CHEM 894 Business skills in the chemical industry**

A review of business skills critical for success of the technical professional in the chemical industry. Topics may include an introduction to financial accounting, organizational design, managing systems, marketing and business strategy, and planning for innovation. 1.5 credit units. Not offered in 2022-2023.

PREREQUISITE: Registration in a graduate program

#### **CHEM 899 Master's Thesis Research**

#### **CHEM 904 Science Leadership and Management**

The Science Leadership and Management course will be delivered over twelve 3-hour sessions to Chemistry and Physics students in either of the first two years of their PhD studies (or other graduate students with permission from the course coordinator and supervisor). The first and last four-week sessions will focus on the development and application of leadership skills, and the second four-week session will focus on the development of management skills, that are useful in scientific positions in industry and academia. To be offered every fall; graded Pass/Fail. Fall. N. Mosey (Coordinator).

EXCLUSION: PHYS 904

#### **CHEM 905 CO2: a scientific & social perspective**

This multidisciplinary course main objective is to learn about the social and scientific concepts behind CO<sub>2</sub> utilization. The participants will learn the basic chemistry of CO<sub>2</sub> and the current ways to sequester and use CO<sub>2</sub> at the laboratory and industrial scales. They will also learn about the impact of CO<sub>2</sub> on society and climate change, the economic advantages of CO<sub>2</sub> utilization and the legal and political aspects related to this modern challenge. This online course will consist of 13 lectures of 2-3 hours given by specialists in the field of CO<sub>2</sub> utilization. They are members and collaborators of the CREATE center on CO<sub>2</sub> utilization and are professors in chemistry, chemical engineering, geological engineering, economy and law. (3.0 credit units).

#### **CHEM 910 Drug Discovery**



The role of the medicinal chemist in industry will be explained by way of lectures covering general drug discovery concepts. A team-based exercise mirroring a real-life drug discovery project will also take place in conjunction with the lectures. Not offered in 2022-2023.

#### **CHEM 912 Green Chemistry**

An introduction to the design of chemical products, reagents, syntheses and solvents for the reduction of the environmental impact of human activities. Design strategies and impact prediction will be emphasized. Offered biannually. Not offered in 2022-2023.

#### **CHEM 913 Organic Free Radical Chemistry**

Structure, stability, persistence, and reactions of organic free radicals; common chain and non-chain radical reactions; mechanisms of initiation, propagation and termination; methods of studying the kinetics of radical reactions; common radical reactions in organic synthesis and applications in natural product synthesis; radicals in biology: lipid peroxidation, radical-trapping antioxidants, radical-based enzymes. Not offered in 2022-2023.

#### **CHEM 914 Asymmetric Synthesis**

Asymmetric hydrogenations and oxidations will be covered with a mechanistic perspective (Nobel prize 2001). Carbon-carbon bond-forming reactions will then be described including nucleophilic additions and cyclopropanations. Asymmetric epoxidation and aziridination will be described. Modern asymmetric reactions including organo catalytic reactions and autocatalytic reactions will also be discussed. Not offered in 2022-2023.

PREREQUISITE: CHEM 863

#### **CHEM 915 Biosynthesis of Natural Products**

This course will examine the biosynthesis of major classes of natural products including polyketides, non-ribosomal peptides, terpenoids, indolocarbazoles, and alkaloids. Focus will be given to the mechanisms of the biosynthetic enzymes. Strategies for discovering new natural products as well as engineering existing pathways to create new compounds will also be considered. Not offered in 2022-2023.

PREREQUISITE: CHEM 883 or equivalent

#### **CHEM 916 Strategies in Total Synthesis**

A discussion of syntheses of complex organic molecules selected from pharmaceutical, natural product, and materials science areas using retrosynthetic analysis concepts. Illustrated syntheses will incorporate fundamentally important and currently significant synthetic methodologies as practiced in small scale academic and process scale industrial laboratories. Not offered in 2022-2023.

PREREQUISITE: CHEM 880

#### **CHEM 917 Microfluidics**

This course will cover subject areas ranging from the fundamentals of microfluidics and nanofluidics suitable for beginners to the examination of applications of microfluidics for end users. A range of devices will be shown and described with various applications ranging from organic synthesis to biochemical analysis. Class participants will learn fabrication and characterization strategies for microfluidic components as well as fluid manipulation and detection methodologies applied to minute volume fluid samples. Not offered in 2022-2023.

#### **CHEM 918 Scanning Probe Methods**

The theory and practice of scanning probe techniques, including scanning tunneling microscopy (STM) and atomic force microscopy (AFM) and related techniques. Applications to modern research in surface and interfacial chemistry. Winter. Z. She.

#### **CHEM 919 Solid State Chemistry**

Introductory solid state theory from the chemist's perspective: free electron metals, Bloch functions and LCAO description of solids. Experimental determination of band structure using photoelectron spectroscopy. Application to material properties such as conductivity, superconductivity, and semiconductors. Winter. P. Wang.

#### **CHEM 920 Photochemistry and Spectroscopy**

Topics include photon absorption, potential energy surfaces and conservation laws, experimental observables and techniques. Laser techniques and molecular beam techniques will be discussed. Laboratory experiments will be related to atmospheric and environmental chemistry. Not offered in 2022-2023.

EXCLUSION: CHEM 841

#### **CHEM 931 Angular Momentum Theory**

Topics include the density matrix formulation, coupling of more than two angular momenta, spherical tensor representations and the Wigner-Eckart theorem. Emphasis will be placed on applications in molecular physics. Not offered in 2022-2023.

#### **CHEM 933 Organic Electronics**

A survey of the basis of molecular electronics, from the molecule properties, to the device behaviour. A critical discussion of organic semiconductors is given in view of its differences with inorganic semiconductors. Future developments such as single molecule devices, molecular sensing and bio-compatible devices are emphasized. Not offered in 2022-2023.

EXCLUSION: CHEM 833

#### **CHEM 936 Advanced Quantum Mechanics**

Topics selected from relativistic electron theory, scattering theory, quantum field theory, wavepacket dynamics,

approximation methods, semiclassical limits, and tunnelling. Not offered in 2022-2023.

EXCLUSIONS: CHEM 930; CHEM 933.

#### **CHEM 937 Advanced Statistical Mechanics**

The application of statistical mechanics to fluids and interfaces. Topics include classical intermolecular and intramolecular potentials, molecular dynamics simulations, Monte Carlo simulations, and analytical theories. Not offered in 2022-2023.

#### **CHEM 938 Density Functional Theory**

An introduction to the techniques and applications of density functional theory. Not offered in 2022-2023.

#### **CHEM 939 Quantum Mechanics in the Continuum**

Most undergraduate quantum courses treat only bound states but much of chemistry occurs in the continuum. This course offers an introduction to the ideas used to understand how molecules fall apart and combine allowing us to apply quantum mechanics to study photodissociation and chemical reactions. Fall. T. Carrington.

#### **CHEM 942 Density Matrix Theory and Spectroscopy**

The theoretical background of density matrix theory and its applications in spectroscopy, particularly multi-dimensional NMR. Not offered in 2022-2023.

#### **CHEM 945 Topics in Interfacial Electrochemistry**

Topics to be covered in this module may include: (a) definition of the electrochemical solid-liquid electrified interface, (b) selected electrochemical techniques (cyclic voltammetry, electrochemical quartz-crystal nanobalance, STM under electrochemical conditions), (c) adsorption at electrode surfaces, (d) under-potential deposition of hydrogen, (e) under-potential deposition of metals, (f) interfacial thermodynamics, and (g) electro-oxidation of noble-metal electrodes. Not offered in 2022-2023.

EXCLUSION: CHEM 845

#### **CHEM 954 Polymer Supramolecular Organization**

Liquid crystalline polymers, spontaneous order and induced order in polymers specifically designed to mimic supramolecular association and recognition. Dendrimers, block structures, and associated surfaces will be included. Winter. G. Liu.

PREREQUISITE: CHEM 984.

#### **CHEM 960 Luminescent Materials Chemistry**

This course introduces the current topics in luminescent materials chemistry including photophysical and photochemical properties of transition metal and main group compounds, and characterization methods. The design and synthetic aspects of luminescent materials and their applications in sensing and optoelectronic devices,

and photocatalysis will also be discussed. Winter. K. Stampeleskie

#### **CHEM 972 Environmental Chemical Sensors**

An overview of chemical sensor and biosensor technology as applied to environmental monitoring. Electrochemical and optical sensors will be discussed, including the fundamental principles behind sensor operation. Performance parameters, such as sensitivity, selectivity, reusability, stability and response will be covered. Detection applications include solvents in air and groundwater, organic contaminants and heavy metals in water and wastewater, and biological contaminants in drinking water. Not offered in 2022-2023.

EXCLUSION: CHEM 872

#### **CHEM 975 Inductively-Coupled Plasma Mass Spectrometry (ICP-MS)**

A detailed description of the technique, means of circumventing its limitations and expanding its capabilities. Examples of applications, including environmental analysis. Not offered in 2022-2023.

#### **CHEM 983 Solving Reaction Mechanisms**

The practical application of basic principles of mechanistic organic chemistry in solving reaction mechanism problems drawn from the chemical literature. Not offered in 2022-2023.

PREREQUISITE: CHEM 882.

#### **CHEM 984 Liquid Crystals**

Fundamental aspects of liquid crystal science at the interface of chemistry and condensed matter physics. Topics will include mesophase structure and characterization, chiral liquid crystals, polymeric liquid crystals, and liquid crystal technology. Not offered in 2022-2023.

#### **CHEM 987 Biomimetic Chemistry**

Topics covered include enzyme models, synzymes, effective molarity, supramolecular chemistry and binding, nucleic acid and peptide mimics, and enzyme inhibitors. Not offered in 2022-2023.

PREREQUISITE: CHEM 886 .

EXCLUSION: CHEM 887.

#### **CHEM 999 Ph.D. Thesis Research**