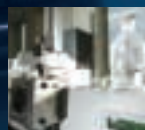
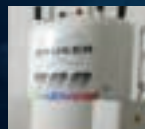


CHEMISTRY RESEARCH INSTRUMENT FACILITIES



INSTRUMENT FACILITIES in the **DEPARTMENT** of **CHEMISTRY** at
McMaster University

INSTRUMENT FACILITIES IN THE DEPARTMENT OF CHEMISTRY AT McMASTER UNIVERSITY

The Department of Chemistry at McMaster University proudly houses three research instrument facilities including the **McMaster Regional Centre for Mass Spectrometry**, the **Nuclear Magnetic Resonance Facility** and the **McMaster Analytical X-Ray Diffraction Facility**. Together, these facilities offer unparalleled service to both internal and external research clients. The combination of state-of-the-art equipment and experienced, professional personnel along with compliance with current good documentation practices (GMP/GLP) allows the staff in the Instrument Facilities to work closely with clients to solve unique problems and provide unrivaled service.

HIGHLIGHTS

- Confidential, personalized service
- All of the Facilities operate under the guidelines of Good Documentation Practices (GMP/GLP)
- Competitive rates for services
- The NMR Facility houses 7 spectrometers, including a Bruker AV 700 and a Bruker AV 600 for biomolecule and small molecule analyses, as well as Bruker AV 500 and AV 300 spectrometers for solid state NMR applications
- The Mass Spectrometry Facility houses 5 instruments capable of small molecule and biomolecule analyses, including a Micromass Quattro Ultima (LC-ESI/APCI Triple Quadrupole MS), a Micromass GCT (EI/CI-TOF MS) and a Micromass Global QTOF Ultima (CapLC ESI/MALDI TOF MS)
- The X-ray Diffraction Facility houses a Mo rotating anode generator with graphite monochromated X-rays for inorganic and organometallic structural studies, as well as a Cu rotating anode generator with a parallel focused beam for organic structure analysis and surface analysis

CONTACT US

Contact us today to arrange a tour of the Instrument Facilities or a presentation of our capabilities at your site!

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Mass Spectrometry ext. 23146
Nuclear Magnetic Resonance ext. 24686
X-ray Crystallography ext. 23107

www.chemistry.mcmaster.ca/facilities

THE NUCLEAR MAGNETIC RESONANCE FACILITY

The Nuclear Magnetic Resonance (NMR) Facility was established in 1985 with funding provided by NSERC and McMaster University. The Facility is equipped with seven NMR spectrometers including the recently acquired Bruker AV 600 and AV 700 spectrometers funded by the Canadian Foundation for Innovation (CFI). The Facility is highly regarded in the Canadian chemical community for its versatility in the types of samples (organic, inorganic, biochemical, geological, industrial, forestry, agricultural and biomedical materials) that can be analyzed. A wide range of nuclei can be studied in solution or in the solid state.

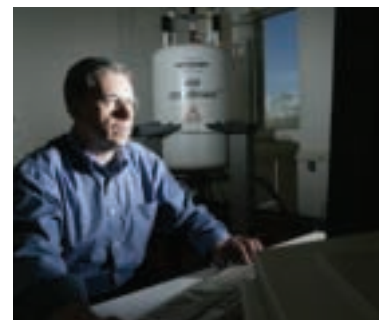
■ Bruker AV 700

The Bruker AV 700 is equipped with an UltraShield Plus magnet and a 5mm inverse triple resonance (TCI-Z) cryoprobe with enhanced sensitivity on ^1H and ^{13}C . It is primarily used for 3-dimensional (3D) structure determination of biomolecules. The spectrometer is located separate from the main NMR Facility in a temperature and humidity controlled environment.



■ Bruker AV 600

This high sensitivity, state-of-the-art instrument is equipped with an UltraShield magnet and an inverse triple resonance multinuclear (TBI-Z) probe. It is used for a variety of 1-dimensional, 2-dimensional and 3-dimensional NMR studies, most prominently structure confirmation and quantitative analysis.

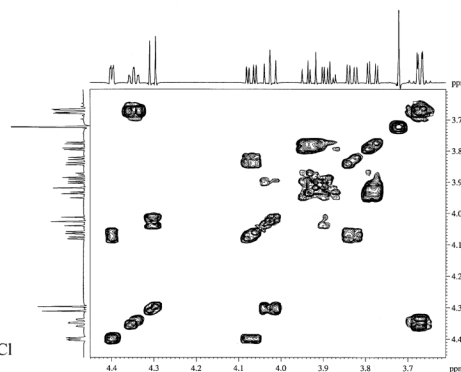
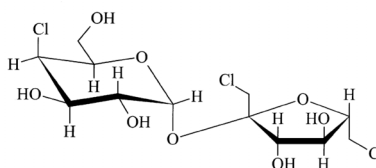


■ Bruker AV 500

The AV 500 is equipped with an UltraShield magnet and high power amplifiers and is primarily used for solid state NMR experiments. Solids probes include 2.5mm, 4mm and 7mm broad band CPMAS (Cross Polarization Magic Angle Spinning) probes with variable temperature capabilities and a 4mm HRMAS (High Resolution Magic Angle Spinning) $^1\text{H}/^{13}\text{C}$ - 2H probe. This instrument is capable of analyzing a wide variety of solid samples with high sensitivity.



2D ^1H - ^1H COSY NMR spectrum of sucralose obtained on the AV 600.



■ THE McMASTER REGIONAL CENTRE FOR MASS SPECTROMETRY

The McMaster Regional Centre for Mass Spectrometry was officially opened in 1986 with funding provided by NSERC and McMaster University. Mass spectrometric service is provided for many clients both within the McMaster community and at external institutions. The staff are willing to undertake service work and project work with individual clients. The combination of state-of-the-art instruments and the expertise of the staff make the Facility one of the best equipped in Canada for the structural elucidation/analysis of unknown organic, inorganic, and biological samples.

■ Waters Micromass Global Ultima

(CapLC ESI/MALDI Quadrupole Time of Flight Mass Spectrometer)

The Global QTOF is interfaced with a capillary LC system for analysis of protein/peptide mixtures. This analysis includes protein/peptide digestion, identification and sequencing. The TOF (time of flight) analyzer provides high resolution (up to 17,500) for accurate mass measurements.



■ Waters Micromass Quattro Ultima

(LC-ESI/APCI Triple Quadrupole Mass Spectrometer)

This state-of-the-art triple quadrupole (QqQ) instrument is dedicated to LC/MS and LC/MS/MS applications using electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI). ESI in particular offers the ability to analyze high molecular mass (up to 100,000 Dalton) compounds and polar or charged species such as peptides, proteins, nucleic acids and nucleotides.



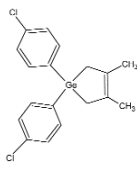
■ Waters Micromass GCT

(EI/CI Time of Flight Mass Spectrometer)

Sample introduction on the GCT instrument occurs using either a probe or a GC interface. The TOF analyzer enables high resolution mass measurements with an accuracy of ~5 ppm on all ions in the spectrum. EI/CI is most suitable for low molecular mass, low polarity compounds (m/z range <1500). The probe may be heated to 650°C to vaporize low volatility compounds.



A high resolution electron ionization mass spectrum of a germanium complex obtained on the Micromass GCT instrument.



■ THE McMASTER ANALYTICAL X-RAY DIFFRACTION FACILITY (MAX)

The McMaster Analytical X-ray Diffraction Facility provides efficient and professional single-crystal and 2-dimensional (2D) powder X-ray analyses at a reasonable cost to clients. The Facility continues to develop advanced techniques and frequently engages in research collaborations. Standard and high resolution X-ray diffraction analyses are both available. Single crystal X-ray analysis provides complete structural characterization including bond lengths, bond angles and torsion angles. Confirmation of stereochemical conformation and absolute configuration are possible, as well as the identification of solvent molecules present in the crystal lattice. This technique can identify polymorphs and isomorphs, and can be used to calculate an ideal powder pattern for comparison to a bulk powder sample. The Facility also contains a high resolution powder diffractometer for characterization of polycrystalline powders and solids. The powder diffraction pattern offers information about sample identification, phase and polymorph characterization and *ab initio* structure solution.

■ Bruker SMART 1K CCD/Mo RA Diffractometer

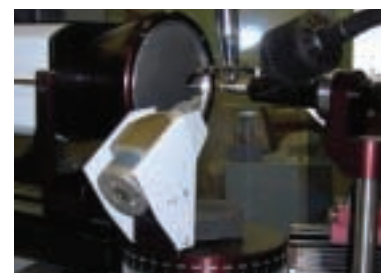
The Facility contains a molybdenum (Mo) rotating anode generator with graphite monochromated X-rays, a 4-circle diffractometer (Bruker P4), and a 2D detector (Bruker Smart1K CCD). This diffractometer is used primarily for inorganic and organometallic single crystal structure determination.



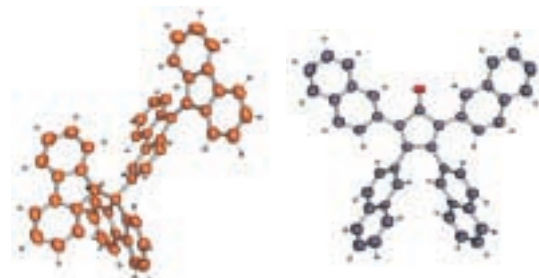
This instrument has also been used for steel and residual stress analyses as well as large crystal orientation determinations.

■ Bruker SMART 6000 CCD/Cu RA Diffractometer

Also contained in the X-ray Facility is a copper (Cu) rotating anode generator (Rigaku) with a parallel focused beam and a 3-circle diffractometer (Bruker D8) with 2D detector (Bruker Smart6000 CCD). This instrument is the most powerful organic small molecule diffractometer in the country! The diffractometer is also used for 2D powder diffraction (rapid phase analysis), fiber diffraction, and texture or strain analyses on films or metal alloys of interest to materials scientists. The instrument also has the potential for observing small angle scattering.



X-ray crystal structures of two organic compounds obtained using the Cu single crystal diffractometer.





CHEMISTRY

INSTRUMENT FACILITIES in the **DEPARTMENT** of **CHEMISTRY** at **McMaster University**

The Facilities in the Department of Chemistry at McMaster University welcome business from other departments, other universities and industrial clients.

Contact us today to arrange a tour or to discuss your research applications and needs.

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