

The A.R. Smith Department of Chemistry Research Instrumentation & Equipment

Laboratories in the A.R. Smith Department of Chemistry are equipped with modern instrumentation which is used regularly by faculty and students:

Analytical Separations and Mass Spectrometry

- **Gas Chromatography Mass Spectrometry (GC-MS)**
 - *Agilent 7890B GC with Leco Pegasus 4D TOF MS*
 - *Agilent 6890 GC with 5973 Quadrapole Mass Analyzer*
 - 70 eV electron ionization with extensive library of compounds
 - Autosampler w/ 100 sample carousel
 - Electron Capture Detector
- **Gas Chromatography with Flame Ionization Detector (GC-FID)**
 - *Agilent 6850 Series II*
 - Autosampler w/ 27 sample carousel
 - Headspace sample introduction with autosampler
- **High Performance Liquid Chromatography (HPLC)**
 - *Dionex UltiMate 3000*
 - 120-vial autosampler
 - Photodiode array (PDA) detector
 - Fraction collector
- **Ion Chromatography (IC)**
 - *Dionex ICS 1000 w/ anion exchange column and conductivity detector*
 - *Dionex ICS 3000 w/ anion exchange column and conductivity detector and electrochemical detector*
- **LC/MS**
 - *Dionex MSQ*
 - Coupled to HPLC or IC
 - Electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) sources
 - Quadrupole mass analyzer

Elemental Analysis

- **Inductively Coupled Plasma Optical Emission Spectrophotometer (ICP-OES)**
 - *Varian 710 ES ICP-OES*
 - Autosampler
 - Axial configuration
 - Simultaneous system for rapid analysis
 - *Perkin Elmer Series II 2400 C,H,N, S,O analyzer*

Molecular Spectroscopy

- **Fourier Transform Infrared (FT-IR) Spectroscopy**
 - *Thermo Scientific Nicolet 6700 FT-IR-Microscope*
 - Accessories for DRIFTS and ATR data collection
 - Resolution: 0.5cm^{-1}
 - *Thermo Scientific Nicolet iS5 FT-IR*
 - Resolution: 0.5cm^{-1}
 - *Shimadzu IRAffinity-1*
 - Accessories for DRIFTS data collection
 - Resolution: 0.5cm^{-1}
- **Raman Spectroscopy**
 - *Enwave Optronics EZRaman*
 - 785 nm diode laser, 300-400 mW
 - Resolution: 6cm^{-1}
 - Spectral coverage: 250 cm^{-1} to 2350 cm^{-1}
 - High sensitivity CCD array
- **Nuclear Magnetic Resonance (NMR) Spectroscopy**
 - *Bruker Avance III HD 400 MHz*
 - Dual broadband probe ($^1\text{H}/^{19}\text{F}$, ^{15}N - ^{31}P)
 - Variable temperature controller
 - Experiments include: COSY, DEPT, HSQC, HMBC, T1-analysis
- **Ultra-violet Visible (UV-Vis) Spectroscopy**
 - *Shimadzu UV-2401 PC double beam spectrophotometer*
 - Frequency range: 190-900nm
 - Resolution: 0.1nm
 - *Shimadzu UV-2600 double beam spectrophotometer*
 - Frequency range: 185-900nm
 - Resolution: 0.1nm
 - *Nanodrop 2000c spectrophotometer*

Fluorescence Spectroscopy

- *Horiba Jobin Yvon FluoroMax-4*
- Xenon arc lamp source
- Excitation and emission monochrometers
- 0.3 nm resolution
- Equipped with 1- and 2-m fiber optic probes, microwell plate reader, and standard 1-cm cuvettes

Fuel Lubricity

- *PCS Instruments High Frequency Reciprocating Rig reciprocating friction and wear test system*
- Fast, repeatable friction and wear measurement
- Microscope with digital camera
- Small, compact bench top system
- Preloaded with standard diesel fuel lubricity test procedures including ASTM D6079
- Built in digital humidity probe

Electrochemistry

- *Bioanalytical Systems (BAS 100B) Electrochemical analyzer*
- Cell stand can accommodate a variety of electrodes
- Hanging mercury drop electrode
- Rotating electrode cell stand

Calorimetry

- *Netzsch DSC 200 F3 Maia Digital Scanning Calorimeter*
- Autosampler and
- Liquid nitrogen cooling.

Computational Quantum Chemistry

- *64-bit PQS computer (equipped with 4 12-core 2.4GHz Xeon processors)*
- This is a 48 core computer with 256 gigabytes of RAM and 16 terabytes of disk storage.
- Supports a variety of quantum chemistry packages including Gaussian09, PQS, GAMESS-US, PSI3, and Cfour. Gaussian09 and its viewer, GaussView5, are available for the windows environment as well.
- Supports a variety of graphical tools including Gabedit, and PQS view
- A large set of methods including semi-empirical, ab-initio (RHF, ROHF, UHF, MCSCF, and CAS-SCF), DFT, MPn, CI, QCI, and coupled-cluster methods can be applied to ground and excited states of molecules

Electrophoresis

- *Beckman Coulter P/ACE MDQ Capillary Electrophoresis System*

Molecular Biology

- *Applied Biosystems - Step One Plus real-time PCR system.*
- *AAPPTEC Focus XC Automated solid phase peptide synthesizer*
- *Tuttnauer 3870 ELV autoclave*