# **Instrumentation in the UCA Chemistry Department**

Hands-on training of students in the operation of these instruments is an essential activity of the department, encompassing instructional and research laboratory experiences. The majority of these instruments are accessible through swipe-Bear-card access, made available when students have been properly trained.

Click on an instrument below to learn more

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Optical (light absorbing) spectrometers	Chromatography, Mass Spectrometry
<ul> <li>Nuclear magnetic resonance (300 MHz FT)</li> <li>Infrared (FT)</li> <li>Raman</li> <li>Electronic (UV-vis-NIR)</li> <li>Nanodrop microvolume spectrometer</li> <li>Electron spin resonance (X-band)</li> <li>Luminescence/fluorescence</li> <li>Atomic absorption (with graphite furnace)</li> </ul>	<ul> <li>MALDI-TOF-Mass Spec.</li> <li>Gas chromatography-Mass Spec.</li> <li>Liquid chromatography-Mass Spec.</li> <li>High Pressure Liquid Chromatography</li> <li>Gel electrophoresis</li> <li>Gas chromatograph</li> </ul>
Additional analytical instrumentation	Specialty application instrumentation
<ul> <li>Scanning potentiostat (CV, coulometry)</li> <li>Digital coulometer</li> <li>Magnetic susceptibility balance</li> <li>Bomb Calorimeter</li> <li>Solution Calorimeter</li> </ul>	<ul> <li><u>Gas-phase ion-molecule reactor</u> (Taylor research lab)</li> <li><u>Cavity-ringdown laser system</u> (Dooley research lab)</li> </ul>
Other specialty equipment	Computational capabilities
<ul> <li><u>Centrifuge</u> (refrigerated)</li> <li>-80 °C freezer</li> <li><u>Speed Vac drier</u></li> <li><u>Inert-atmosphere glovebox</u></li> <li><u>Microwave synthesizer</u></li> </ul>	<ul> <li>Macbook's (18) running Gaussian suite</li> <li><u>Mini-mainframe</u> (Long research lab)</li> </ul>
The department is also well-equipped with:	
pH meters, melt-temps, Spec 20's, circulating chillers, roto-evaporators, smaller	

centrifuges, etc.

### Nuclear Magnetic Resonance (NMR) Spectrometer back to top JEOL ECX-300 FT

NMR is among the most powerful techniques for the determination of the structures of molecules. Using the magnetic signals generated by spinning atomic nuclei, the same physical phenomenon used for medical MRI imaging, the instrument provides

a wide variety of structural information particularly the proximity of different parts of a molecule to one another. Our JOEL 300 MHz instrument allows spectra to be determined for a wide variety of different atomic nuclei and is capable of performing all of the many modern NMR experiments developed over the past 25 years including COSY, HMQC, and NOSY. The instrument was funded by an NSF grant written by Dr. Jerry Manion.



### Infrared Spectrometer back to top Nicolet iS50 FT

Infrared spectroscopy measures the absorption of infrared light resulting from the internal motion of molecules (bond vibrations and rocking/scissoring of bonds). It is

an important technique in the identification of compounds. Our instrument can analyze solids (KBr pellets, ATR), liquids, and gases. This specific instrument was acquired through an NSF EPSCoR award to Dr. D Perry.



### Raman Spectrometer <u>back to top</u> Advantage 633

Raman is a vibrational spectroscopy tool like infrared, but one that differs in how molecules are induced to respond. Raman uses visible light to excite vibrations. It complements IR measurements, and works with samples less accessible to conventional IR, like aqueous solutions. This was acquired through an NSF RUI award to Dr. Don Perry.



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# **Electronic (UV-vis-NIR) Spectrometer**

Agilent Cary 60 (x 2 instruments)

Electronic spectroscopy measures the absorption of ultra violet-visible-and near IR light by molecules. It is a tool to probe the structure and concentration of proteins (UV light). It is also widely used to study the electronic structure of transition metal ions and organic molecules. The department also has a diffuse reflectance attachment for this instrument enabling spectra of solid samples to be readily measured in the visible region.



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## **Electron Spin Resonance Spectrometer**

Resonance Instruments 8400 (X-band)

ESR (or EPR) is a tool that studies systems with unpaired electrons using a magnet and microwave radiation. The signals it receives from spin flipping of these electrons gives information about the immediate environment of these electrons in the material. ESR is a readily applied to solids (like rubies, clay, and rice bran), liquids, and gases (like NO<sub>2</sub>).

### Luminescence Spectrometer back to top Perkin Elmer LS 45

Fluorescence is a process of light emission by molecules widely used to detect molecules in very low concentrations and to probe the structures of large biomolecules. This particular instrument is equipped with a stopped-flow accessory allowing for the observation of luminescence emissions from fast chemical reactions.



### Atomic Absorption Spectrometer <u>back to top</u> Buck Scientific 210VGP and 220GF graphite furnace

Atomic Absorption spectroscopy is used to measure the amount of a metal ion present in a solution. The instrument can reach metal ions in very low (ppm, ppb) concentrations. It is particularly valuable in studying metal pollution in natural

samples (like mercury in Lake Ouachita fish) and in natural waters (e.g. lead in Flint drinking water or well-water). The graphite furnace accessory allows the system to reach extremely trace low concentrations of these ions



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### Gas Chromatography-Mass Spectrometer Varian Saturn 2200 GC-MS

GC-MS combines the power of gas chromatography in separating the components of a mixture of volatile compounds with the power of mass spectrometry to identify each of the individual components. One major use is its use in verifying the composition of substances suspected of containing illegal drugs. The purchase of this instrument was funded by an NSF grant authored by Dr. Donald Perry.

# Liquid Chromatography-(TQ)Mass Spectrometer

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Waters Acquity LC-TQMS

Similar to the GC-MS in that liquid chromatography is used to separate compounds in a mixture and the triple quad mass spectrometer is used to identify them. This instrument can be used with nonvolatile samples such as those typically found in biological samples or natural samples, like well-water and chemically digested dirt samples. The triple quad detector provides a number of detector options.





### MALDI – Time-of-Flight Mass Spectrometer <u>back to top</u> Micromass MicroMX

This instrument uses Matrix Assisted Laser Desorption/ionization to generate ions

that are then analyzed by Time-Of-Flight mass spectrometry. MALDI produces low energy ions which remain intact and are then characterized using the time-offlight spectrometer. It is especially valuable for use with large molecular weight molecules (proteins and polymers) that are unstable when analyzed by more conventional techniques. Both this instrument and the LC-TQMS were acquired through an NSF grant written by Dr. Cameron Dorey. Most recently Dr. Dunlap is using this in her biochemistry research and teaching labs, to characterize proteins with molar masses of over 8000-10,000 g/mol.

### High Pressure Liquid Chromatography Waters M6000A with PDA detector

This instrument is essentially the front half of the LC-MS instrument mentioned above. HPLC is ideally suited for separation and isolation of a number of biologically active compounds including lipids, steroids, plant pigments, and many pharmaceuticals. Since many of these compounds are conjugated, the PDA detector allows for a range of wavelengths to be detected simultaneously. This is a key instrument in use in Dr. Kelley's laboratory where they

focus on separation, isolation and identification of natural and synthetic derivatives of vitamin A.

### Gas Chromatography Gow-Mac Series 400

This basic GC instrument is used for routine analysis in the instructional organic labs and is also used by various research groups. Like most modern instrumentation, it is equipped with a digital data acquisition system that allows the results to be processed by a computer.

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### Cyclic Voltammetry / Coulometry <u>back to top</u> EG&G Model 362 (potentiostat) / Electrosynthesis 680 (dig. coulometer)

Cyclic Voltammetry is an electroanalytical technique that provides information about electrochemical reactions such as reduction potentials, numbers of electrons

involved, and reversibility of redox processes. Coulometry is a companion technique, where the coulometer "counts" electrons transferred in a redox process. This can provide quantitative electrochemical information about a chemical system.

# Magnetic Susceptibility Balance

Johnson Matthey MSB-1

This instrument is used to measure the paramagnetic properties of substances that result from unpaired electrons they contain. It is particularly well suited to analyze transition metal complexes. This magnetic information is related to both the numbers of valence electrons a metal ion possesses and the immediate chemical environment of the metal ion in the sample.

### Inert Atmosphere Glovebox back to top MBraun Unilab

Samples that are sensitive to air require special handling techniques that include this glove box, which contains a dry, inert nitrogen gas atmosphere. This box is also equipped with a -30 °C freezer and is plumbed to allow purified and dried solvents to be piped directly into the inert atmosphere chamber.







### **Microwave Synthesizer**

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### CEM Discover with Explorer autosample changer

The use of microwaves in place of traditional thermal heating (like oil or sand baths) to facilitate chemical synthesis has become increasingly common in recent years. Just like warming food in your kitchen, reaction times using this instrument are greatly reduced (from hours to minutes in most cases), increasing the efficiency of effort spent in the classrooms that use it (organic and inorganic labs) and research labs. The cavity of the CEM is sized so as to also accept small round-bottom flasks for larger reaction volumes.

# Vacuum apparatus/solution concentrator

ThermoSci - Speedvac DPD121P

The equipment enables dissolved species to be isolated from solutions by evaporating the solvents away in a controlled environment. This is used in biochemical and analytical applications where analytes of interest are extracted from samples being tested. Analytes isolated using this tool can then be identified and quantified use some of the myriad other instrumentation described in this summary.

### **Centrifuge (refrigerated)** Beckman J2-HS

This high speed/high volume instrument is used to separate cells from solutions as well as biochemical components of cell contents.



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### Bomb Calorimeter Parr

This instrument allows for the very precise measurement of calorie content in materials, including combustible compounds, foodstuffs (chips, cookies, etc.), and even in minnows that are natural foods of game fish. This device measures the heat produced when these materials are combusted in a pure oxygen atmosphere

# **Solution Calorimeter**

Parr L45IEB

This is a companion tool to the bomb calorimeter. It very precisely measures the heat change associated with chemical processes that happen in solution, from the dissolving of solids to the reactions of acids and bases.

# **Gas Phase Ion-Molecule Reaction Apparatus**

Taylor research: modified MS, glow discharge ion source and ion optics

This instrument is used in Dr. Taylor's lab to study fundamental chemical processes occurring between metal ions and neutral molecules. In this device, metal ions are formed in a distribution of electronic states using a sputtering glow discharge (similar to a neon light) and subsequently injected into a drift cell containing a mixture of He and a small amount of the neutral reactant. Products of these reactions are then analyzed using a quadrupole mass filter. The

drift cell can also be used to determine the relative amounts of excited and ground state metal ions using a technique called electronic state chromatography, which distinguishes the different states on the basis of their mobilities in He gas. If carried out in the presence of the reactive neutral, a variation on this technique can be used to determine state-specific products and reaction kinetics.

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### **Cavity-ringdown** laser system

Dooley research equipment

Dr. Dooley uses this equipment to study light-scattering by atmospheric particles, including clumps of liquid drops (aerosols and clouds) and dust. This provides fundamental physical measurements of how particles scatter light in the Earth's atmosphere, and it can be used to quantify the amounts of these particles present. The cavity-ringdown component allows her lab to simulate long distances (hundred's of meters) associated with light moving through the atmosphere but in a small laboratory space.

# Mini-mainframe/Gaussian suite (Linux)

Long research: MicroHPC2 16-core

This computer system is used by Dr. Long's research lab to simulate interactions between DNA and other groups, like metal ions and molecules. She also uses the Gaussian suite of programs to model the internal electronic structure of molecules that are the interest of her's and other research groups in the department.

## Nanodrop microvolume spectrometer

Dunlap research: NanoDrop 1, ThermoFisher

This spectrometer records electronic spectra (UV-vis) using microvolume samples (only 1-2  $\mu$ L). Dr. Dunlap uses this to record UV absorptions for her protein samples. The software translates the absorbance into a normalized value if the path length was a typical 1 cm cell.





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