

John C. Wright Andreas C. Albrecht Professor of Chemistry

Department of Chemistry

1101 University Avenue Madison, Wisconsin 53706

Syllabus for Chemistry 621

Chemistry 621- Experimental Spectroscopy- This 4-credit class meets each week for three 50-minute lectures and one 4 hour laboratory (optional). Over the course of the semester, students are expected to do at least 90 hours of learning activities, which includes class attendance, reading, studying, preparation, problem sets, and other learning activities. The course is based on a complete set of notes, research publications, and computer programs that simulate fundamental principles underlying chemical instrumentation. Python is required for all homework.

Course Description- The theory behind current instrumental methods employed in chemical analysis with applications in spectroscopy, electrochemistry, chromatography, electrophoresis, mass spectroscopy, and nuclear magnetic resonance. **Requisites:** none

Instructor- Andreas Albrecht Professor of Chemistry John C. Wright. Office hours at 10-11 AM on Monday and Tuesday or by student stopping in. Contact via wright@chem.wisc.edu, telephone 608-262-0351, or visiting office (room 3209).

Course Designation: Breadth - Physical Science. Course counts toward the Natural Science requirements.

Course URL - https://canvas.wisc.edu/courses/105459

Meeting Time and Location- M,W,F at 8:50 AM in room 2377.

Instructional mode: face-to face

Level – Advanced

L&S Credit Information - Counts as Liberal Arts and Science credit in L&S. 4 credits with lab; 3 credits without lab. The credit allocation follows the Traditional Carnegie Definition – One hour (i.e. 50 minutes) of classroom or direct faculty/instructor instruction and a minimum of two hours of out of class student work each week over approximately 15 weeks, or an equivalent amount of engagement over a different number of weeks. The 3 hour laboratory counts as 1 credit.

Grad 50% - Counts toward 50% graduate coursework requirement

Repeatable for Credit: No

Course Instructor- Professor John C. Wright, office 3209 Chemistry, Office Hours 10-11 AM on Mondays and Tuesdays, phone is 608-262-0351, wright@chem.wisc.edu.

Course Website URL- https://canvas.wisc.edu/courses/76146

Three weekly lectures-8:50-9:40 AM on Monday, Wednesday, and Friday

FAX: (608) 262-0453 wright@chem.wisc.edu TEL: (608) 262-0351

Laboratory Sections- One 3 hour laboratory meeting. Five sections that are scheduled each day of the week.

Course objectives- This course's objectives are to present complete coverage of all of the topics that are required for a Ph.D. level experimental analytical scientist. The course covers the fundamental experimental and theoretical foundations of spectroscopy, electrochemistry, separations, mass spectroscopy, and nuclear magnetic resonance. The course requires students to quantitatively master the theoretical foundations underlying the each topic using Python software.

Course Learning Outcomes- Students finishing this course will have the knowledge and skills to perform instrumental chemical analysis.

Requirements, Grading, and Evaluation- Students will do weekly assignments that require development of theoretical simulations of theory and experimental methodologies for each course topic, and read and analyze current instrumental research publications. Students will deliver their work to the course website dropbox, present their work to the class at weekly homework discussion sections and the individual students will grade their own work. Final exam will be given at the end of the course. Relative weights will be determined in consultation with class.

Academic Integrity

By enrolling in this course, each student assumes the responsibilities of an active participant in UW-Madison's community of scholars in which everyone's academic work and behavior are held to the highest academic integrity standards. Academic misconduct compromises the integrity of the university. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these acts are examples of academic misconduct, which can result in disciplinary action. This includes but is not limited to failure on the assignment/course, disciplinary probation, or suspension. Substantial or repeated cases of misconduct will be forwarded to the Office of Student Conduct & Community Standards for additional review. For more information, refer to studentconduct.wiscweb.wisc.edu/academic-integrity/.

Accommodations for Students with Disabilities

McBurney Disability Resource Center syllabus statement: "The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform faculty [me] of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Faculty [I], will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA." http://mcburney.wisc.edu/facstaffother/faculty/syllabus.php

Diversity & Inclusion

Institutional statement on diversity: "Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the

profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals.

The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world." https://diversity.wisc.edu/

The lecture schedule appears below:

9/4 Labor Day 9/6 Light and Simple Optics 9/9 Photomultipliers and Absorption Measurements 9/11 Emission measurements; Instruments; Lineshapes 9/13 Nature of Light 9/16 Diffraction and Interference 9/18 Laser beams and diffraction gratings 9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics 10/9 Infrared and Raman Spectroscopy; X-Ray and Photoelectron Spectroscopi	
9/6 Light and Simple Optics 9/9 Photomultipliers and Absorption Measurements 9/11 Emission measurements; Instruments; Lineshapes 9/13 Nature of Light 9/16 Diffraction and Interference 9/18 Laser beams and diffraction gratings 9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/9 Photomultipliers and Absorption Measurements 9/11 Emission measurements; Instruments; Lineshapes 9/13 Nature of Light 9/16 Diffraction and Interference 9/18 Laser beams and diffraction gratings 9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/11 Emission measurements; Instruments; Lineshapes 9/13 Nature of Light 9/16 Diffraction and Interference 9/18 Laser beams and diffraction gratings 9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/13 Nature of Light 9/16 Diffraction and Interference 9/18 Laser beams and diffraction gratings 9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/16 Diffraction and Interference 9/18 Laser beams and diffraction gratings 9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/18 Laser beams and diffraction gratings 9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/20 Gratings and Monochromators 9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/23 Monochromators 9/25 Microscopes, laser beam profiles, focusing lasers 9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/27 FTIR and Fourier transforms 9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
9/30 Fourier transforms and resolution 10/2 Introduction to Electronic and Vibrartional Spectroscopy 10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
10/4 Vibrational and Electronic Spectroscopy 10/7 Molecular dynamics	
10/7 Molecular dynamics	
10/9 Infrared and Raman Spectroscopy: X-Ray and Photoelectron Spectroscopi	es
10/11 X-Ray and Photoelectron Spectroscopies and Eloectrochemistry	
10/14 Potentiometry and Voltammetry	
10/16 Fundamentals of Potentiometry	
10/18 Fundamentals of Voltammetry	
10/21 Voltammetry- Diffusion Controlled	
10/23 Voltammetry- Kinetic Controlled, Marcus Theory	
10/25 Pulsed Voltammetry, Photovoltaics and Photocatalysis	
10/28 Chromatographic Fundamentals and Gas Chromatography	
10/30 Gas Chromatography and HPLC	
11/1 HPLC and Electrophoresis	
11/4 Electrophoresis	
11/6 Introduction to Mass Spectroscopy	
11/8 Quadrupole Mass Spectroscopy	
11/11 TOF & Quadrupole MS	
11/13 Time of Flight Mass Spectroscopy	
11/15 FTMS & Magnetic and Electric Sector MS	
11/18 Orbitrap	
11/20 MS3 & Other MS Methods	
11/22 Ionization Methods	
11/25 Introduction to NMR	
11/27 Rotating Frame	
11/29 Thanksgiving Break	
12/2 NMR Exercises, J-J coupling	
12/4 Decoupling, inversion recovery, spin echo	
12/6 J modulation and population transfer	
12/9 Population transfer, INEPT	
12/11 2D NMR, COSY, HMQC, HSQC	
12/13 Study Day	
12/14 Final Examination- 7:45-9:45	