Instrumental Analysis

CHEM 221 (graduate)

Instructor Info

David Punihaole, PhD

TBD

Innovation Hall E352

David.Punihaole@uvm.edu

Course Info

CHEM 121

MWF

08:30 - 09:20

VOTEY 305

Overview

This 3-credit course presents a survey of instrumental methods of chemical analysis. Students are expected to draw upon knowledge from previous courses they have taken, including General Chemistry, Quantitative Analysis, Introductory Physics, and Calculus. We will focus on understanding the fundamental principles underlying different methods and their realization in modern instrumentation for chemical analysis. We will focus on the following broad methodological areas:

- Spectroscopy
- Chromatography
- Mass Spectrometry
- Electrochemistry

This is not a "how-to" course. You will not learn how to operate analytical instruments nor will we cover specific analytical "recipes." These change (sometimes quite quickly) with time as the discipline grows, so our focus on principles and concepts of implementation should provide greater insight both into how current instruments work as well as the basis for your understanding how they will work a decade from now. Lastly, we will pay attention to the chemical systems to which these methods are applicable and how best to obtain the chemical information desired using the most appropriate instrumental methods.

Learning Objectives

This course fulfills core competencies in analytical/critical thinking and quantitative reasoning/applied data interpretation. You should develop an understanding of the analytical capabilities of a number of instrumental methods and be able to suggest suitable instrumental methods for particular problems in chemistry. To choose the best instrumental method for addressing an analytical chemistry problem, we will consider:

- the property or quantity of the chemical system to be measured
- the physical and chemical principles upon which the measurement is based
- generation of a signal by a suitable detector (transducer) and the processing of the signal to convert it to a form appropriate for a readout device
- the strengths and limitations of each particular instrumental method

To make these kinds of assessments, you will need to assess:

- the chemical and/or physical principles exploited during the measurement
- how the instrument actually makes the measurement, and
- some of the techniques used to improve analytical figures of merit (such as accuracy, precision, and sensitivity).

Course Philosophy

Each of us approaches science with a different perspective informed by our personal upbringing, educational background, socioeconomic status, racial identity, ethnicity, and gender. My goal is to create a classroom environment that supports students from a diverse set of backgrounds. I strongly believe that our best path forward to making scientific progress is to promote inclusiveness and equality. It is my expectation that every member of this class will also support diversity and inclusion. As a community, we should strive to uphold the ideals of Our Common Ground and welcome any suggestions as to how I can promote a more diverse and inclusive classroom.

Required Texbook

Principles of Instrumental Analysis - 7th Ed. by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 9781305577213)

Available at the UVM Book Store, Amazon, or the publisher, Cengage.

Grading Scheme

Grading Scale

40%	Exams, 10% each
10%	Paper
10%	Presentation
30%	Projects, 10% each
10%	Attendance/Participation

Grades will follow the standard scale: A+ > 96-100%; A > 92-96%; A- > 89- 92%; B+ > 87- 89%; B > 82- 86%; B- > 79- 82%; C+ > 76- 79%; C > 72- 76%; C- > 69- 72%; D+ > 66- 69%; D > 62- 66%; D- > 60- 62%; F < 60%. Grades will be curved at the discretion of the professor. Please note: undergraduate and graduate students will be grading separately with different grading curves.

Assessments of Graded Work

- Exams: Exams are take-home. Unless otherwise noted, you will have a week to complete the exams. Exams will be primarily conceptual in nature. They will be designed to test mastery and understanding of the material at a deep-level. Calculators are not necessary, but will be allowed. Exams will be open book/open notebook, and students will be allowed to work in groups of their choosing. Exams will typically be 4 or 5 questions, which will typically require short essay responses. Please note that exams will test students on anything covered in the textbook or in class. Late exams will not be accepted unless otherwise excused by me.
- Paper: All graduate students in CHEM 221 must write a 5-page paper covering recent advancements in an analytical method. The topic will be chosen in consultation with me. You will be expected to provide a review of the current state of research in that field and critically assess at least five journal articles published within the last five years. Your critique assess the utility of the method in different applications, weighs its strengths and weaknesses, and compare it to traditional or gold-standard techniques.
- Presentation: All graduate students in CHEM 221 must give an oral presentation on their chosen paper topic. Students are expected to introduce the method and present a brief history of its development. Students must also assess the utility of the method in different applications, weigh its strengths and weaknesses, and compare it to traditional or gold-standard techniques. Students are expected to field questions from the audience.
- Projects: There will be three coding-based projects assigned during the semester. These projects are designed to allow students to study certain topics covered in class in deeper detail and may require rudimentary knowledge of coding. You may use any programming language or numerical computing environment to answer coding-related problems. Please speak to me if you do not have coding experience or require help to answer these or other problems. Projects will be due on assigned dates specified in the syllabus at 22:00. Late project assignments will not be accepted unless otherwise excused by me. Rubrics specifying grading criteria will be provided to the students on the date that the projects are formally assigned in class.
- Attendance/Participation: During 10 randomly selected lectures, attendance will be taken or class participation will be assessed.

Course Format

Modality Description

This course will be held in-person unless otherwise specified.

Blackboard and Microsoft Teams

Important course announcements will be posted on Blackboard. The use of laptops, iPads, and other mobile devices to follow/make class notes and participate in course activities is highly encouraged. Please speak to me if this is not possible for you. Please refrain from using these devices for anything but activities related to the class.

Course Policies

General Attendance, Participation Policies, and Expectations

Attendance/participation in this course is expected for you to succeed. Students are expected to show up on time at the start of class. I reserve the right to ask students to leave the classroom if they are being disruptive or are chronically late to class. The UVM attendance policy outlines expectations for attendance. Students are expected to complete homework and read relevant chapters in the book (which will be posted prior to lecture) before class. Science has never and is not done in isolation. A major part of this course will depend upon class discussion, working in teams, or participating in other group activities. Students are expected to be teamplayers and to maintain a respectful learning environment so that everyone is heard. Racist, sexist, or any other bigoted language will not be tolerated and are grounds for being asked to leave the class. Finally, given the content-heavy nature of this course, it is virtually impossible to cover every topic in the course notes in detail. Course lectures will be reserved for covering what I deem to be the most important or difficult topics. However, any material covered in the course notes are fair game for exams or homework assignments.

Excused Absence Policies

- Religious Holidays: Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of your absence to me in writing by the end of the second full week of classes. You will be permitted to make up work within a mutually agreed-upon time frame. https://www.uvm.edu/registrar/religious-holidays
- Inter-collegiate Athletics: Members of UVM varsity and junior varsity teams are responsible for documenting in writing any conflicts between their planned athletic schedule and the class schedule by the end of the 2nd full week of classes. You will be permitted to make up work within a mutually agreed-upon time frame.
- Medical and Emergency Absences: Absences due to sickness, as well as medical and family emergencies, should be brought to my attention as soon as possible. You will be permitted to make up work within a mutually agreed-upon time frame.
- Other Absences: Absences due to extracurricular or other activities not specified above should be brought to my attention as soon as possible so that we can work out an arrangement to make up work.

Email Policy

Students are encouraged to email me directly to clarify any questions concerning homework, projects, or materials covered in the course. The subject line of emails should only contain the words "CHEM 221" (please keep exact formatting). Emails will be filtered using this subject line to ensure that they are not mistakenly missed. I will not respond to emails that do not contain these words in the subject line. Unless there is an emergency, I will generally only answer students' emails once a day, at around 18:30. I expect students to respond or acknowledge my emails to them within 48 hours of sending.

Important University Policies

Academic Integrity

Offenses against the Code of Academic Integrity are deemed serious and insult the integrity of the entire academic community. Any suspected violations of the code are taken very seriously and will be forwarded to the Center for Student Ethics and Standards for further investigation. Violations of the Code of Academic Integrity–including any inappropriate collaboration, collusion, cheating, corroboration, plagiarism, or any other related offense–will be fully investigated according to the rules set by the UVM Academic Integrity Office and may be punishable with a score of zero for the assignment in question. Details can be found at

http://www.uvm.edu/policies/student/acadintegrity.pdf.

Grade Appeals

If you would like to contest a grade, please follow the procedures outlined in this policy:

https://www.uvm.edu/policies/student/gradeappeals.pdf

Code of Student Conduct

http://www.uvm.edu/policies/student/studentcode.pdf

FERPA Rights Disclosure

The purpose of this policy is to communicate the rights of students regarding access to, and privacy of their student educational records as provided for in the Family Educational Rights and Privacy Act (FERPA) of 1974.

http://catalogue.uvm.edu/undergraduate/academicinfo/ferparightsdisclosure/

Promoting Health and Safety

The University of Vermont's number one priority is to support a healthy and safe community:

Center for Health and Wellbeing https://www.uvm.edu/health

Counseling & Psychiatry Services (CAPS): Please call 802-656-3340 for assistance.

C.A.R.E.: If you are concerned about a UVM community member or are concerned about a specific event, we encourage you to contact the Dean of Students Office (802-656-3380). If you would like to remain anonymous, you can report your concerns online by visiting the Dean of Students website at https://www.uvm.edu/studentaffairs

Alcohol and Cannabis Statement

As a faculty member, I want you to get the most you can out of this course. You play a crucial role in your education and in your readiness to learn and fully engage with the course material. It is important to note that alcohol and cannabis have no place in an academic environment. They can seriously impair your ability to learn and retain information not only in the moment you may be using, but up to 48 hours or more afterwards. In addition, alcohol and cannabis can:

- Cause issues with attention, memory and concentration
- Negatively impact the quality of how information is processed and ultimately stored
- Affect sleep patterns, which interferes with long-term memory formation

It is my expectation that you will do everything you can to optimize your learning and to fully participate in this course.

Student Resources

Technical support for students

Students, please read this technology checklist to make sure you are ready for classes. Students should contact the Helpline (802-656-2604) for support with technical issues.

Research and Citation Help

For help selecting research topics, finding information, citing sources, and more, ask a librarian. Although they are working remotely, librarians are always eager to help. You may ask questions by phone, e-mail, chat, or text, or make an appointment for an individual consultation with a librarian.

- Howe Library: https://library.uvm.edu/askhowe
- Dana Medical Library: https://dana.uvm.edu/help/ask
- Silver Special Collections Library: https://specialcollections.uvm.edu/help/ask

Student Learning Accommodations

In keeping with University policy, any student with a documented disability interested in utilizing accommodations should contact SAS, the office of Disability Services on campus. SAS works with students and faculty in an interactive process to explore reasonable and appropriate accommodations, which are communicated to faculty in an accommodation letter. All students are strongly encouraged to meet with their faculty to discuss the accommodations they plan to use in each course.

Contact SAS:
A170 Living/Learning Center
802-656-7753
access@uvm.edu
https://www.uvm.edu/access

Diversity, Equity, and Inclusion Resources

The Division of Diversity, Equity, and Inclusion Center believes excellence should be inclusive of the entire University of Vermont (UVM) community and is steadfastly committed to this belief. Every day, our Division strives to make our work accessible, affirming, and action-oriented to help ensure excellence is inclusive of everyone.

https://www.uvm.edu/diversity

UVM Prism Center

The Prism Center serves the diverse queer and trans communities at the University of Vermont. We support and empower lesbian, gay, bisexual, transgender and queer students, as well as students whose identities fall in between or expand beyond those categories, and work to create a campus community where people of all sexual and gender identities can thrive.

https://www.uvm.edu/prism

Interfaith Center

Each of us engages those questions differently, perhaps through a religious tradition, philosophy, or spiritual practice. No matter how you make meaning of your life, you are welcome at the Interfaith Center for reflection, spiritual practice, education, and community building.

https://www.uvm.edu/interfaithcenter

Mosaic Center for Students of Color

The Mosaic Center for Students of Color (MCSC) Vision is to create a diverse and rich community of empowered, engaged, and enthusiastic students of color at UVM. We fully support the holistic development of self-identified students of color so that they can obtain their goals for academic achievement, personal growth, identity formation, and cultural development.

https://www.uvm.edu/mcsc

Women & Gender Equity Center

The UVM Women & Gender Equity Center cultivates a joyful community while advancing gender equity across identities. We envision a brave, diverse, and equitable learning environment for all members of the UVM community. We provide advocacy services for those in our community who have experienced sexual or intimate partner violence, and strive to provide programming, education, and events that ask our community to explore the intersections of their gender and other identities.

https://www.uvm.edu/wagecenter

Tips for Success

Students are encouraged to attend class, do homework, come to office hours, work with peers, and ask questions to help them succeed in class. In case the course goes fully online, here are a few resources for students on remote/online learning:

- Checklist for success in: https://learn.uvm.edu/about/support-for-students/checklist-online-credit-courses/
- Academic support for online courses: https://www.uvm.edu/academicsuccess/online-learning-student-resources-remote-instruction

Helpful resources other than the instructor include the Undergraduate/Graduate Writing Center, Supplemental Instruction, Learning Co-op tutors, and supplemental course materials.)

Course Schedule (Subject to Change)

Electronics, Signal and Noise

Jan 18	Lecture 1	Syllabus, Introduction
Jan 20	Lecture 2	Overview and Choice of Analytical Methods
Jan 23	Lecture 3	Calibration of Instrumental Methods, Performance Characteristics
Jan 25	Lecture 4	Ohm's & Kirchoff's Laws, Intro to Electronics
Jan 27	Lecture 5	Intro to Electronics (cont'd) (select 3 candidate papers for graduate project)
Jan 30	Lecture 6	Signal and Noise
Feb 1	Lecture 7	RC Circuits & Analog filtering
Feb 3	Lecture 8	Operational Amplifiers (finalize selection of paper for graduate project)

(Molecular) Optical Spectroscopy

Feb 6	Lecture 9	Lock-in amplification, Digital Signal-to-Noise Enhancement (Exam 1, Project 1 Due)
Feb 8	Lecture 10	Characteristics of Electromagnetic Radiation
Feb 10	Lecture 11	Sources of Electromagnetic Radiation, Mirrors, Prisms
Feb 13	Lecture 12	Spectrometers, Detectors (Exam 1 Due)
Feb 15	Lecture 13	Theory of spectral lineshapes (virtual lecture)
Feb 17	Lecture 14	Beer's Law, UV-Vis Absorption Instrumentation (virtual lecture)
Feb 20		President's Day
Feb 22	Lecture 15	Deviations from Beer's Law
Feb 24	Lecture 16	Effects of Noise on UV-Vis Spectrophotometric Analysis
Feb 27	Lecture 17	UV-Visible Spectroscopy Applications
Mar 1	Lecture 18	Intro to IR Absorption Spectroscopy (guest lecture by Rusul Mustafa)
Mar 3	Lecture 19	Fourier Transform and Attenuated Total Reflectance IR
Mar 6	Lecture 20	Theory of Raman Scattering
Mar 8	Lecture 21	Different Flavors of Raman Spectroscopy
Mar 10	Lecture 22	Raman Instrumentation
Mar 13		Spring Recess
Mar 15		Spring Recess
Mar 17		Spring Recess

Nuclear Magnetic Resonance Spectroscopy & (Molecular) Mass Spectrometry

Mar 20	Lecture 23	Infrared/Raman Spectroscopy Applications (guest lecture) (Exam 2, Project 2 Due)
Mar 22	Lecture 24	Theory of Nuclear Magnetic Resonance (guest lecture by Dr. Monika Ivancic)
Mar 24	Lecture 25	Environmental Effects on Chemical Shift (guest lecture by Dr. Monika Ivancic)
Mar 27	Lecture 26	Spectral Integration, Spin-Spin coupling (submit first draft of paper)
Mar 29	Lecture 27	NMR Instrumentation
Mar 31	Lecture 28	NMR Spectroscopy Applications (Part 1) (Exam 2 Due)
Apr 3	Lecture 29	NMR Spectroscopy Applications (Part 2)
Apr 5	Lecture 30	Intro to Molecular Mass Spectrometry, MS Sampling & Ionization Methods
Apr 7	Lecture 31	Ionization Methods (cont'd), Mass Analyzers
Apr 10	Lecture 32	Mass Analyzers (cont'd), Transducers
Apr 12	Lecture 33	Molecular Mass Spectrometry Applications
Apr 14	Lecture 34	Tour of NMR, ALCA, and Raman facilities (Exam 3)

Chromatography

Apr 17	Lecture 35	Introduction to Separations, Retention Factor, Partition Coefficient
Apr 19	Lecture 36	Selectivity Factor, Band Broadening, Column Efficiency
Apr 21	Lecture 37	Theory of Band Broadening, Column Resolution, Band Separation (Exam 3 Due)
Apr 24	Lecture 38	Gas Chromatography
Apr 26	Lecture 39	HPLC Chromatography
Apr 28	Lecture 40	Chromatography Applications (Project 3 Due, Papers Due)
May 1	Lecture 41	Graduate Student Presentations (Part 1)
May 3	Lecture 42	Graduate Student Presentations (Part 2)
May 5	Lecture 43	Graduate Student Presentations (Part 3) (Exam 4)