CHEM 226: Analytical Spectroscopy

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Fall 2020

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Office Hours: T 16:00 - 18:00 (MS Teams) or By Appt.
Class Room: Votey Hall Rm. 207

Class Hours: T/R 13:15-14:30
Office: Innovation Hall E352
Credits: 3.00

Course Prerequisites

Instrumental Analysis (CHEM 221)

Course Description and Learning Objectives

In this course, you will learn the fundamental concepts and principles of optical spectroscopic methods of analysis. Emphasis will be placed on fundamental theoretical concepts, instrumentation and practices, as well as applications of molecular spectroscopic methods. This course aims to establish a rigorous foundation (without delving deep into quantum mechanics) to understand fundamental aspects of different optical spectroscopies such as UV and IR absorbance, Rayleigh and Raman scattering, as well as sophisticated non-linear techniques such as Sum Frequency Generation, Coherent Anti-Stokes Raman, and Stimulated Raman. To accomplish this, we will examine, from a first principles perspective, toy models (e.g. the Lorentzian model of the atom) and the theories that underlie various phenomena (e.g. absorption, dispersion, and polarization) that form the basis of different optical spectroscopies. By the end of the course, students should be able to: 1) quantitatively describe the theories that underlie different optical spectroscopy methods; 2) explain how different measurements are made and the instrumentation required; 3) determine their utility in different real-world analytical chemistry applications; and 4) critically evaluate scientific literature in the field of analytical spectroscopy.

Modality description

Given the small class size, this course will be held in-person unless otherwise specified. Students attending lecture must obey strict social distancing requirements and other UVM policies as stipulated by the university's Green and Gold Promise. I will give students instructions on how to proceed in the event that the course switches to an online-only format due to COVID-19 concerns.

Recommended Course Materials:

There is no required textbook for this course, but several are recommended:

- Alan Marshall, *Biophysical Chemistry*, John Wiley & Sons, Inc., 1976.
- Jeanne L. McHale, *Molecular Spectroscopy (2nd Ed.)*, CRC Press, 2017.
- James D. Ingle and Stanley R. Crouch *Spectrochemical Analysis*, AbeBooks, 1988.
- Max Diem *Introduction to Modern Vibrational Spectroscopy*, John Wiley & Sons Inc., 1993.
- Robert W. Boyd *Nonlinear Optics (3rd Ed.)*, Academic Press, Inc., 2008.

Copies of chapters belonging to recommended textbooks can be made available upon request to me. These copies are for educational purposes only. Please do not distribute these copies.

Blackboard and Microsoft Teams

Class notes will be posted to Blackboard. Microsoft Teams will be used in the event that this course switches to an online-only format. 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.

Attendance Policy and Classroom Environment Expectations

General Attendance, Participation Policies, and Expectations

Attendance/participation in this course is expected and accounts for a percentage of your grade. The UVM attendance policy outlines expectations for attendance. Students are expected to complete homework and read class notes (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.

COVID-specific Policies

The University of Vermont reserves the right to make changes in the course offerings (http://catalogue.uvm.edu/), mode of delivery, degree requirements, charges, regulations, and procedures contained herein as educational, financial, and health, safety, and welfare considerations require, or as necessary to be compliant with governmental, accreditation, or public health directives.

Due to COVID-19 concerns,students are expected to maintain a safe atmosphere when attending class. The Green and Gold Promise clearly articulates the expectations that UVM has for students, faculty, and staff to remain compliant with all COVID-19 recommendations from the federal CDC, the State of Vermont, and the City of Burlington. This include following all rules regarding facial coverings and social distancing when attending class. If you do not follow these guidelines, I will ask you to leave the class. If

you forget your mask, you cannot enter the class and should go back and retrieve your mask. The Code of Student Conduct outlines policies related to violations of the Green and Gold Promise. Sanctions for violations include fines, educational sanctions, parent notification, probation, and suspension.

You may need to isolate or quarantine this semester due to COVID-19 concerns. If this is the case, Student Health Services will inform the Dean's office. I will then contact the dean's office for confirmation that a student is in quarantine or isolation. Students, especially those who are asymptomatic in quarantine, will be expected to continue their academic work. I will work with students in quarantine and isolation in a mutually agreed-upon format to make-up missed course material and attend lecture virtually. Students are encouraged to email me directly to discuss how to proceed in the course during quarantine/isolation. All course notes and readings will be available to the student on Blackboard.

Email Policy

Students are encourage 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 226: Analytical Spectrocopy." Emails will be filtered using this subject line to ensure that they are not mistakenly missed. Unless there is an emergency, I will only answer students' emails twice a day, at around 08:30 and 18:30.

Grading Criteria/Policies

- **Graded Components:** Midterm (10%), Final (10%), Homework (40%), Projects (35%), Participation/Attendance (5%)
- **Late Policy:** Late work will not be accepted unless excused by me. The university policy on incomplete grades is located at .
- **Grading Scale:** The typical UVM grading scale will be used. This is a small course, so there is no reason why students should not all be able to receive good grades! I roughly aim to award the top 30 - 50% of students in the class an "A." The remainder of the class will receive a "B" grade in the class. Any grade lower than a "B-" will be awarded in cases where the student consistently fails to do homework or project assignments. I reserve the right to curve the grading scale depending on overall class scores at the end of the semester. Any curve will only ever make it easier to obtain a certain letter grade. Undergraduate and graduate students will be held to different grading scales.

Assessments (Graded Work)

- **Midterm and Final Exams:** The midterm and final exams will be primarily conceptual in nature. No calculators will be needed or allowed. I may make the exams take-home due to COVID-19 related concerns.
- **Homework:** The largest portion of the grades will be weighted towards homework. Homework assignments will be graded on a completion or best effort basis. It is entirely acceptable and encouraged to work with your peers on the weekly problem sets. The problem sets will consist of between 3 - 10 problems 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. Homework will be assigned on Tuesdays and will be due the following Thursday. Late assignments will not be accepted unless otherwise excused by me.
- **Projects:** There will be two projects assigned during the semester. These projects are designed to expose students to primary literature in the field of analytical spectroscopy, as well as cultivate their scientific writing and oral presentation skills. For the first project, students will be asked to write an essay that critically analyzes a scientific paper. I will give students feedback on their essays, and they will be given an opportunity to revise their papers for additional points. For the second project, students will be asked to give a presentation that critically analyzes another scientific paper. Students will work on the second project in groups, but will be graded on an individual basis. Late 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.
- **Participation/Attendance:** Students are encourage to actively engage with the material covered in class in the form of questions, contributing to discussions, and attending office hours.

Recording Class Sessions

Our class sessions may be audiovisually recorded for students in the class to refer back to, and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate orally are agreeing to have their voices recorded. If you are not willing to consent to have your voice recorded during

class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live.

Technical support for students

Students, please read this technology check list 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

Course Evaluation

All students are expected to complete an evaluation of the course at its conclusion. The evaluations will be anonymous and confidential so that students may speak candidly about their experiences. The information gained, including constructive criticisms, will be used to improve the course.

Intellectual Property Statement

Students are prohibited from publicly sharing or selling academic materials that they did not author (for example: class syllabus, outlines or class presentations authored by the professor, practice questions, text from the textbook or other copyrighted class materials, etc.); and students are prohibited from sharing assessments(for example homework or a take-home examination). Violations will be handled under UVM's Intellectual Property policy and Code of Academic Integrity.

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 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 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 encourage 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.)

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.

Course Schedule and weekly learning goals

The schedule is tentative and subject to change. The topics listed below are teaching goals and should be viewed as the key concepts you will learn during each week, and also as a study guide before each exam, and at the end of the semester. Each exam will test on the material that was taught up until 1 week prior to the exam. The topics covered in the second half of the semester tend to build on the concepts in the first half of the semester, so it is still important to at least review those concepts throughout the semester.

Week 01, 08/31 - 09/04: Harmonic Oscillator

- Topic 1: Syllabus Introduction, Mass-on-a-spring problem
- Topic 2: Introduction to Electricity and Magnetism

Week 02, 09/07 - 09/11: Electromagnetic Radiation

- Topic 1: Electrostatics, Dipole Moment, Polarizability
- Topic 2: Polarization, Electric Susceptibility

Week 03, 09/14 - 09/18: Absorption and Dispersion

- Topic 1: Absorption vs. Dispersion
- Topic 2: Absorption (cont.), Circular Dichroism

Week 04, 09/21 - 09/25: Elastic Light Scattering

- Topic 1: Rayleigh vs. Thomson Scattering
- Topic 2: Static Light Scattering

Week 05, 09/28 - 10/02: Raman (Inelastic) Scattering

- Topic 1: Introduction to Raman Spectroscopy
- Topic 2: Surface and Tip-enhanced Raman spectroscopy

Week 06, 10/05 - 10/09: Applications of Spectroscopic Techniques

- Topic 1: Applications of Raman Spectroscopy
- Topic 2: TBD

Week 07, 10/12 - 10/16: Midterm Exam Week

- Midterm Review/Class Discussion (10/13)
- **Project 1 Assigned (10/13)**
- **Midterm Exam (10/15)**

Week 08, 10/19 - 10/23: Non-linear Spectroscopy

- Topic 1: Three-Wave Mixing Processes
- Topic 2: Four-Wave Mixing Processes

Week 09, 10/26 - 10/30: Coherent Raman Scattering

- Topic 1: Stimulated and Coherent Anti-Stokes Raman Scattering
- Topic 2: Applications of Coherent Raman Spectroscopy
- **Project 1 Due (10/29)**

Week 10, 11/02 - 11/06: Lasers and Optical Setups

- Topic 1: Reflective and Refractive Optics
- Topic 2: Lasers and optical setups
- **Project 2 Assigned (11/3)**

Week 11, 11/09 - 11/13: Detecting/Measuring Signals

- Topic 1: Diffraction and Spectrometers
- Topic 2: Interferometry and Detectors
- **Project 1 revisions due (11/12)**

Week 12, 11/16 - 11/20: Signal-to-Noise Analysis

- Topic 1: Introduction to Signal and Noise
- Topic 2: Signal amplification and Noise filtering

Week 13, 11/23 - 11/27: Class Discussion and Fall Break

- Final Review/Class Discussion (11/24)

Week 14, 11/30 - 12/04: Final Presentations

- **Project 2 Group Presentations (12/1) and (12/3)**