

CHEMISTRY 8152  
Bruinicks 123  
MWF 9:05am – 9:50am

Prof. Renee R. Frontiera  
Office: Smith 233  
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# **ANALYTICAL SPECTROSCOPY**

## **FALL SEMESTER 2017, 4 CREDITS**

CHEM 8152 is a graduate level course which explores the fundamental principles of analytical spectroscopy. This course also encourages you to think creatively about current scientific problems. I'd like for you to end the semester ready to optimally use analytical spectroscopic techniques, based on an understanding of the physical phenomena behind by each method, the way an instrument works under ideal conditions, as well as the non-ideal behavior and limitations of each technique.

The objectives for this course are:

- (1) Identify appropriate spectroscopic techniques for analysis of any sample. Recognize the strengths and limitations of each technique.
- (2) Critically evaluate scientific literature and seminars in the area of analytical spectroscopy. Ask meaningful questions while exploring a new topic.
- (3) Devise a novel research project which uses analytical spectroscopic methods to explore an important unanswered question. Recognize the previous work and identify state-of-the-art work in your chosen area.

### **COURSE OVERVIEW:**

The first unit of the course will cover the fundamental principles of analytical spectroscopy, including light sources, optical setup and detection schemes, and signal generation and analysis. We will then look at the interaction of visible and infrared light with matter, progressing from atoms to molecules to plasmonic materials. The final unit of the course will focus on techniques including NMR and ultrafast spectroscopies.

### **OPTIONAL TEXTBOOK:**

James D. Ingle, Jr. and Stanley R. Crouch, "Spectrochemical Analysis", 1988, ISBN 0138268762

### **SUPPLEMENTAL READING:**

Eugene Hecht, "Optics", Addison Wesley, 2002, ISBN-10: 0805385665

J. Michael Hollas, "Modern Spectroscopy", Wiley, 2004, ISBN-10: 0470844167

Douglas Skoog, "Principles of Instrumental Analysis", Brooks Cole, 2006, ISBN-10: 0495012017

**OFFICE HOURS:** Mondays 10-11, or anytime by appointment. Send me an email to set up a time if you'd like to meet. I'm happy to talk about anything relating to the course, or things outside of the course, like graduate school or the University of Minnesota.

**TEACHING ASSISTANT:** Our TA for the course is graduate student Siu Yi Kwang, [kwang005@umn.edu](mailto:kwang005@umn.edu). She's available for office hours by appointment, or is happy to set up a regular office hour on request.

### GRADING:

Midterm 1 (Oct 20, in class)	100 pts	20%
Midterm 2 (Dec 19, 1:30 pm)	100 pts	20%
Problem sets (5)	75 pts	15%
Proposal	150 pts	30%
Minute papers (10)	75 pts	15%

### EXAMS:

There will be two midterm exams during the semester, one during class on October 20<sup>th</sup> and the other on Dec 19<sup>th</sup> at 1:30 pm (the date of the final). Each midterm is worth 100 points. A calculator (without internet access!) will be helpful for both exams. You may bring a one-sided 8.5" x 11" page of equations and notes to each midterm exam.

### PROBLEM SETS:

Each of the five problem sets will be worth 15 points. Feel free to work together on the problem sets, but every person must submit their own unique solutions, showing all your work. All of the problem sets are due by 5pm in my mailbox (B-18, near 139 Smith). Assignments submitted late without prior arrangement will not be graded.

### MINUTE PAPERS:

The purposes of "minute papers" are to get you reading and thinking critically about the scientific literature as well as seminars offered in the department. Minute papers are short evaluations of a recent journal article or seminar, accepted within the last two months. There will be ten minute papers due throughout the semester, worth 15% of your final grade. To get started, there are two things you should do:

1. Check out the Chemistry Department seminar schedule ([chem.umn.edu/seminar/](http://chem.umn.edu/seminar/))
2. Sign up for ASAP alerts or RSS feeds for journals relevant to the class. Good options are *JACS*, *Analytical Chemistry* or *Journal of Physical Chemistry (A, B, C, and/or Letters)*. If you are having trouble signing up for ASAP alerts, make sure you are on campus or accessing the internet through the VPN.

Every week you will either attend a seminar or read a new article from a journal that is relevant to this class. Then, you'll write a short summary (short = readable in a minute). You should discuss the spectroscopic technique used, the major findings, and your ideas about what the work is lacking or what could be done next. Please keep your papers under 500 words. Minute papers will be due Friday at 5pm, and need to be submitted to the class's Moodle page – feel free to read minute papers from your classmates!

Of the ten minute papers due, *at least two of them must be based on a seminar*. In the Chemistry Department, Eric Potma's seminar on Sept 14<sup>th</sup>, Keith Nelson's seminar on October 10<sup>th</sup>, Naomi Halas' seminar on October 12<sup>th</sup>, and Cynthia Friend's seminars on Oct 31<sup>st</sup> and Nov

2<sup>nd</sup> are especially encouraged. If you find other seminars in other departments with an emphasis on spectroscopy, let me know and I will post on Moodle! Sometimes there will be themes for the minute papers, but if you go to a seminar it's ok if it doesn't fit the weekly theme.

The grading breakdown for minute papers is as follows:

1.5 pts = description of the spectroscopic technique

1.5 pts = description of the findings

3 pts = evaluation of the work/future ideas

1.5 pts = grammar/writing style/length

## **PROPOSAL**

The proposal will consist of three parts: a white paper, an experimental outline, and a presentation. Each person will propose an unexplored chemistry research question and choose appropriate spectroscopic methods to investigate this problem.

### **White paper:**

A white paper is commonly the first step in applying for a research grant. Granting agencies use white papers (relatively short) to determine who will be invited to submit full research proposals (much longer).

The white paper for your research proposal is limited to **two pages** including any figures, single-spaced, 12 pt font, 1 inch margins. References may be included on additional pages.

Your white paper should address the following topics:

-Background/context: what is the problem to be addressed and why is it important?

-Objective: what do you plan to accomplish in a three-year program?

-Rationale: what is the value of this work to the scientific community and/or general public?

-Technical approach: what is your strategy for addressing this problem?

-Anticipated outcome: if successful, what exactly will you have learned?

-Estimated costs: what amount of funding are you requesting per year and why?

\*\*White paper guidelines adapted from Prof. Christy Haynes and <http://www.src.org>.

### **Experimental Outline:**

Your outline is limited to **two pages** and should detail exactly the experiments that would be done each year to perform the proposed research. Make sure to discuss sample preparation, control experiments, analysis technique, and an overall proposed timeline.

### **Presentation:**

Each person will present their research proposal to the rest of the class. Please prepare a 10 minute presentation – either electronic presentations or “chalk talks” are fine. If you choose an electronic presentation, please send your presentation to Prof. Frontiera by email by 5pm on the day before your presentation. Please let me know two days before your presentation if you would like to use a format other than .pptx, .ppt, or .pdf.

The grading rubric for the proposal is as follows:

**White paper: 75 points**

10 points each for bullet points listed above

5 points: writing/organization

10 points: creativity, originality, feasibility of proposed project

**Experimental Outline: 25 points**

10 points: Sample preparation and description of chosen technique(s)

5 points: Control experiments

5 points: Timeline

5 points: Writing, rational design

**Presentation: 50 points**

10 points: Organization (audience appropriate, logical sequence, all terms defined)

15 points: Content (introduction is attention grabbing, accurate information, appropriate amount of material relevant to overall message, clear conclusion)

15 points: Presentation style (eye contact, clear voice, practiced, appropriate length)

10 points: Thoughtfulness and quality of evaluations, asking questions during presentations

**POLICIES**

Please see:

[http://policy.umn.edu/Policies/Education/Education/SYLLABUSREQUIREMENTS\\_APPA.html](http://policy.umn.edu/Policies/Education/Education/SYLLABUSREQUIREMENTS_APPA.html)

for information on UMn policies including student conduct, disability accommodations, sexual harassment, and others. Students registered with disability services should contact Dr.

Frontiera as soon as possible to discuss accommodations outlined in their letter.

**SCHOLASTIC DISHONESTY ([policy.umn.edu/education/syllabusrequirements-appa](http://policy.umn.edu/education/syllabusrequirements-appa))**

You are expected to do your own academic work and cite sources as necessary. Failing to do so is scholastic dishonesty. Scholastic dishonesty means plagiarizing; cheating on assignments or examinations; engaging in unauthorized collaboration on academic work; taking, acquiring, or using test materials without faculty permission; submitting false or incomplete records of academic achievement; acting alone or in cooperation with another to falsify records or to obtain dishonestly grades, honors, awards, or professional endorsement; altering, forging, or misusing a University academic record; or fabricating or falsifying data, research procedures, or data analysis. (Student Conduct Code:

[http://regents.umn.edu/sites/default/files/policies/Student\\_Conduct\\_Code.pdf](http://regents.umn.edu/sites/default/files/policies/Student_Conduct_Code.pdf)) If it is

determined that a student has cheated, he or she may be given an "F" or an "N" for the course, and may face additional sanctions from the University. For additional information, please see:

<http://policy.umn.edu/Policies/Education/Education/INSTRUCTORRESP.html>.

## **COURSE TOPICS**

1. Light sources and lasers
2. Optics and diffraction
3. Detectors
4. Super-resolution microscopy
5. Atomic spectroscopy
6. Molecular absorption and emission, FRET
7. Curve fitting
8. IR and 2D-IR
9. Raman, including resonance Raman, stimulated Raman and surface-enhanced Raman
10. TBD: NMR, ultrafast spectroscopy, etc