

Chemistry 513
Analytical Molecular and Atomic Spectroscopy

Course Information for Spring 2019

Class Meeting Days/Times: M, W, F 9:55AM-10:45AM

This course will use a combination of synchronous (via WebEx), asynchronous (recording and reading via Canvas) and, possibly, in-person lectures. Please see announcements in Canvas.

Class Location: Please see important announcement in Canvas. If in-person lectures are announced, class will meet in Gilman 1312.

Prerequisites: *Undergraduate Instrumental Analysis, Undergraduate Quantum Mechanics*

- Check the course's Canvas page for announcements, assigned reading, and other course content

Instructor Information

Emily Smith
 Office: Gilman 0706
 Email: esmith1@iastate.edu

- Appointments welcomed, please make an appointment to meet with me via WebEx

Resources

Assigned literature reading can be obtained in Canvas (most are also available online through the library)

Most lecture notes will be posted to Canvas. You are encouraged to use these notes as an electronic resource

Course Grades and Exam Policies

Exam 1	<u>February 26, 2021*</u>	20%
Exam 2	<u>April 5, 2021*</u>	20%

*take-home exam with an indicated due date (February 26 or April 5)

Final Exam	<u>May 5, 9:45 to 11:45 AM**</u>	30%
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** additional details to be announced

Class participation, attendance		30%
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Class Preparation and Conduct

- It is to your benefit to participate in classroom discussions and ask questions!
- Students creating disturbances that interfere with the conduct of the class or the learning of others will be asked to leave the lecture room and/or removed from WebEx.

Topics Not Covered in this Course

Mass Spectrometry (see Chemistry 577)

Specific Surface Sensitive Spectroscopies (see Chemistry 576)

Spectral Identification of Organic Compounds (see Chemistry 572)

In-depth Quantum Mechanical description of Spectroscopy (see Chemistry 562 & 564)

All links below are to external websites.

Academic Misconduct

The class will follow Iowa State University's policy on academic dishonesty. Anyone suspected of academic dishonesty will be reported to the [Dean of Students Office](#). Academic Misconduct in any form is in violation of Iowa State University *Student Disciplinary Regulations* and will not be tolerated. This includes but is not limited to: copying or sharing answers on tests or assignments, plagiarism, submitting a lab report for an experiment not performed, and having someone else do your academic work. Depending on the act, a student could receive an F grade on the test/assignment, F grade for the course, and could be suspended or expelled from the University. See the Conduct Code at www.dso.iastate.edu/ja for more details and a full explanation of the Academic Misconduct policies.

All work submitted for this class in your name must be your own. In the event that you use work from books and any other source to complete your work it must be **properly cited**. Copying from any source without proper reference is considered plagiarism (http://instr.iastate.libguides.com/understanding_plagiarism) and will be reported to the Dean of Students.

Accessibility Statement

Iowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. Students requesting accommodations for a documented disability are required to work directly with staff in Student Accessibility Services (SAS) to establish eligibility and learn about related processes before accommodations will be identified. After eligibility is established, SAS staff will create and issue a Notification Letter for each course listing approved reasonable accommodations. This document will be made available to the student and instructor either electronically or in hard-copy every semester. Students and instructors are encouraged to review contents of the Notification Letters as early in the semester as possible to identify a specific, timely plan to deliver/receive the indicated accommodations. Reasonable accommodations are not retroactive in nature and are not intended to be an unfair advantage. Additional information or assistance is available online at www.sas.dso.iastate.edu, by contacting SAS staff by email at accessibility@iastate.edu, or by calling 515-294-7220. Student Accessibility Services is a unit in the Dean of Students Office located at 1076 Student Services Building.

Harassment and Discrimination

Iowa State University does not discriminate on the basis of race, color, age, ethnicity, religion, national origin, pregnancy, sexual orientation, gender identity, genetic information, sex, marital status, disability, or status as a U.S. Veteran. Inquiries regarding non-discrimination policies may

be directed to Office of Equal Opportunity, 3410 Beardshear Hall, 515 Morrill Road, Ames, Iowa 50011, Tel. 515-294-7612, Hotline 515-294-1222, email eooffice@iastate.edu

Religious Accommodation

Iowa State University welcomes diversity of religious beliefs and practices, recognizing the contributions differing experiences and viewpoints can bring to the community. There may be times when an academic requirement conflicts with religious observances and practices. If that happens, students may request the reasonable accommodation for religious practices. In all cases, you must put your request in writing. The instructor will review the situation in an effort to provide a reasonable accommodation when possible to do so without fundamentally altering a course. For students, you should first discuss the conflict and your requested accommodation with your professor at the earliest possible time. You or your instructor may also seek assistance from the [Dean of Students Office](#) at 515-294-1020 or the [Office of Equal Opportunity](#) at 515-294-7612.

Freedom of Speech and Academic Freedom

Iowa State University supports and upholds the First Amendment protection of [freedom of speech](#) and the principle of [academic freedom](#) in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.

Contact Information

If you are experiencing, or have experienced, a problem with any of the above issues, email academicissues@iastate.edu

Schedule and assigned reading on the following pages.

Tentative Schedule & Assigned Reading

Month	Day	Topic	Assigned Literature reference #
			#:chapter
Jan	25	Electromagnetic Radiation	1:Sections 1.1 and 1.2 pages 1-8
	27	Signal, Noise, Background, Error	2 pages 135-154
	29	Signal, Noise, Background, Error	3
Feb	1	Instrumentation: Optics	4: Chapter 4 pages 86-104
	3	Instrumentation: Optics	4: Chapter 5 pages 149-196
	5	Instrumentation: Optics	4: 6.3 pages 253-273
	8	Instrumentation: Sources	1: Chapter 2
	10	Instrumentation: Lasers	5: Chapter 9.1 and 9.2 pages 337-362
	12	Instrumentation: Monochromator/spectrometer	1:Chapter 3.1 & 3.2; 2:pages 60-75
	15	Instrumentation: Monochromator/spectrometer	1:Chapter 3.1 & 3.2; 2:pages 60-75
	17	Instrumentation: Detectors	1:Chapter 3.3 pages 82-105; 6
	19	Instrumentation: Detectors	1:Chapter 3.3 pages 82-105; 6
	22	Atomic Spectroscopy: Introduction, line spectra	8 pages 1 to 28
	24	Atomic Spectroscopy: Introduction, line spectra	2:Sections 7-3 and 7-4
	26	EXAM 1	
Mar	1	Atomic Spectroscopy: AAS/AES	2: Chapter 10 pages 273-280
	3	Atomic Spectroscopy: AAS/AES	2: Chapter 8 pages 225-243
	5	Molecular Spectroscopy: Introduction	2: Chapter 12
	8	Molecular Spectroscopy: Introduction	Finish 2: Chapter 12
	10	Molecular Spectroscopy: UV-visible spectrophotometry	2: (pages 352-365)
	12	Molecular Spectroscopy: Beer's Law/circular dichroism	2: (pages 372-381); 11
	15	Molecular Spectroscopy: Infrared	2: Chapter 14
	17	Molecular Spectroscopy: Fourier Transform	12; 13; 14
	19	Molecular Spectroscopy: Luminescence	2: Chapter 15
	22	Molecular Spectroscopy: Luminescence	15
	24	Molecular Spectroscopy: Luminescence	16
	26	Molecular Spectroscopy: Luminescence	17; 18
	29	Molecular Spectroscopy: Raman Scattering	19: Chapters 1 & 2; 2: (pages 494-510)
	31	Molecular Spectroscopy: SERS & Resonance Raman	20; 21; 22
April	2	Molecular Spectroscopy: Nonlinear Spectroscopy	23; 24
	5	EXAM 2	
	7	Molecular Spectroscopy: Nonlinear Spectroscopy	25
	9	Spatial Resolution and Imaging	26; 27
	12	Imaging	28
	14	Subdiffraction imaging	29; 30; 31
	16	Surface Plasmons	32
	19	Molecular Spectroscopy: Reflection: SPR	33; 34
	21	Molecular Spectroscopy: photoacoustic spectroscopy	35
	23	Spectral Data analysis: Calibrations, background, noise	36; 37; 38
	26	Spectral Data analysis: Autocorrelation	39
	28	Spectral Data analysis: Chemometrics	41; 42; 43
	30	Spectral Data analysis: Machine Learning	none
May	5	Final Exam 9:45 - 11:45 AM	

Literature reading (“File name on Canvas”):

- #1 Garcia Sole, J.; Jaque, D. "An Introduction to the Optical Spectroscopy of Inorganic Solids" John Wiley & Sons Ltd. **2005**.
- #2 Ingle, J.D.; Crouch, S. R. "Spectrochemical Analysis" Prentice Hall **1988**.
- #3 Ursula Hofacker, "Chemical Experimentation: An integrated course in inorganic analytical, and physical chemistry" W. Freeman 1972.
- #4 Hecht, E. "Optics" Pearson, **2002**, 4th Edition.
- #5 Hollas, J.M. Modern Spectroscopy Fourth Edition Chapter 9 "Lasers and Laser Spectroscopy" John Wiley & Sons Ltd. 2004.
- #6 Sweedler, J.V. et al., "High Performance Charge Transfer Device Detectors" *Anal. Chem.* Vol 60, No. 4, 1988 pg. 282A.
- #7 None, note there isn't a listing for 7
- #8 Herzberg, G. "Atomic Spectroscopy and Atomic Structure" Dover Publications **1944**.
- #9 Fortes et al. "Laser-Induced Breakdown Spectroscopy" *Anal. Chem.* 2013 85, 640-669.
- #10 Pfeil, D. "Measurement Techniques for Mercury: Which Approach is Right for You?" IET September/October 2011.
- #11 Li et al. "Method to Determine Protein Concentration in the Protein-Nanoparticle Conjugates Aqueous Solution Using Circular Dichroism Spectroscopy" *Anal. Chem* 2015, 87, 6455-6459.
- #12 Faires, L.M. "Fourier Transform for Analytical Atomic Spectroscopy" *Anal. Chem.* Vol. 58 No. 9 **1986** 1023A-1034A.
- #13 Horlick, G. "Fourier Transform Approaches to Spectroscopy" *Anal. Chem.* Vol. 43 No. 8 **1971** 61A-66A.
- #14 Perkins, W.D. "Fourier Transform-Infrared Spectroscopy" *J. Chem. Ed.* Vol. 63 No. 1 **1986** A5-A10.
- #15. Hellen Ishikawa-Ankerhold, Richard Ankerhold and Gregor Drummen "Advanced Fluorescence Microscopy Techniques—FRAP, FLIP, FLAP, FRET and FLIM" *Molecules* **2012**, 17, 4047-4132.
- #16 Ulai Noomnarm, Robert M. Clegg "Fluorescence lifetimes: fundamentals and interpretations" *Photosynth. Res.* Vol. 101 **2009** pg. 181–194.
- #17 Neuweiler, H. "Exploring Light by Single Molecule Fluorescence Spectroscopy" *Analytical Chemistry* **May 1, 2005** 179A.
- #18 Li, J.; Zhu, J.-J. "Quantum Dots for Fluorescent Biosensing and Bio-imaging Applications" *Analyst* **2013**, 138, 2506.
- #19 Richard McCreery "Raman Spectroscopy for Chemical Analysis" John Wiley & Sons, Inc., **2000**
- #20 Andrzej Kudelski "Analytical applications of Raman spectroscopy" *Talanta* 76 **2008** pg. 1–8.
- #21 Haynes, C.L. et al "Surface Enhanced Raman Spectroscopy" *Analytical Chemistry* **September 1, 2006** 339A (see A page articles).
- #22 Iwamoto, R.; Ohta, K.; Miya, M.; Mima, S. "Total Internal Reflection Raman Spectroscopy at the Critical Angle for Raman Measurements of Thin Films" *Applied Spectroscopy* Vol. 35 No. 6 **1981** pg. 584-587.
- #23 Blanchard, G.J. "Time-resolved and Short-Pulse Laser Spectroscopies" *Applied Spectroscopy* Vol. 55 No. 3 **2001** 110A.
- #24 Swofford and Albrecht "Nonlinear Spectroscopy" *Ann. Rev. Phys. Chem.* **1978**. 29:421-40.
- #25 Ji-Xin Cheng "Coherent Anti-Stokes Raman Scattering Microscopy" *Applied Spectroscopy* Volume 61, Number 9, **2007** pg. 197A.
- #26 Wolf, D.E., "The Optics of Microscope Image Formation I." *Methods Cell Biol.* Vol 81, **2007** pg. 11-42.
- #27 Jennifer C. Waters "Accuracy and precision in quantitative fluorescence Microscopy" *J. Cell Biol.* Vol. 185 No. 7 **2009** pg. 1135–1148.
- #28 Schlcker, S. "Raman Microspectroscopy: A Comparison of Point, Line and Wide-Field Imaging Methodology: *Analytical Chemistry* 75(16) **2003** 4312-4318.
- #29 George H. Patterson "Fluorescence microscopy below the diffraction limit" *Seminars in Cell & Developmental Biology* Vol. 20 **2009** pg. 886–893.
- #30 Boris B. Akhremitchev, Steven Pollack, and Gilbert C. "Apertureless Scanning Near-Field Infrared Microscopy of a Rough Polymeric Surface" *Langmuir* **2001**, 17, 2774-2781.
- #31 Blom et al. "Stimulated Emission Depletion Microscope" *Chemical Reviews* 2017 117, 7377-7427.

- #32 Dean J. Campbell, Younan Xia "Plasmons: Why Should We Care?" *Journal of Chemical Education* Vol. 84 No. 1 January **2007** pg. 91.
- #33 Ekgasit, S.; Thammacharoen, C.; Yu, F.; Knoll, W. "Evanescent Field in Surface Plasmon Resonance and Surface Plasmon Field-Enhanced Fluorescence Spectroscopies" *Anal. Chem.* Vol. 76 **2004** pg. 2210-2219.
- #34 Abdennour Abbas, Matthew J. Linman, Quan Cheng "Sensitivity comparison of surface plasmon resonance and plasmon-waveguide resonance biosensors" *Sensors and Actuators B* 156 (**2011**) 169–175.
- #35 Haisch, C. "Photoacoustic Spectroscopy for Analytical Measurements" *Meas. Sci. Technol.* **2012**, 23 012001.
- #36 Vickers et al. "Curve Fitting and Linearity: Data Processing in Raman Spectroscopy" *Applied Spectroscopy* 2001 55, 389.
- #37 Lieber et al. "Automated Method for Subtraction of Fluorescence from Biological Raman Spectra" *Applied Spectroscopy* 2003 57, 1363.
- #38 Simpson and Harris "Raman Spectroscopy of the Liquid-Solid Interface: Monolayer and Bilayer Adsorption of Pyridine on Silica" *J. Phys. Chem.* 1990 94, 4649-4654.
- #39 Schwille, P.; Haustein, E; "Fluorescence Correlation Spectroscopy" *Biophysics Textbook Online*.
- #40 Thompson, N.L.; Pero, J.K. "Total Internal Reflection Fluorescence Correlation Spectroscopy" *Reviews in Fluorescence* Vol. 3 **2006** pg. 215-237.
- #41 Cooper, J.B. "Chemometric Analysis of Raman Spectroscopic Data for Process Control Applications" *Chemometrics and Intelligent Laboratory Systems* **1999** 46, 231-247.
- #42 Bro et al. "Principal Component Analysis" *Analytical Methods* 2014 6, 2812-2831.
- #43 Leger and Ryder "Comparison of Derivate Preprocessing and Automated Polynomial Baseline Correction Method for Classification and Quantification of Narcotics in Solid Mixtures" *Applied Spectroscopy* 60, 182.

The instructor reserves the right to make changes to the syllabus and will notify students of any changes in lecture and Canvas when possible.