CHEMISTRY 547-Special Topics In Analytical Chemistry

APPLIED INFRARED SPECTROSCOPY: FUNDAMENTALS, TECHNIQUES, AND ANALYTICAL PROBLEM-SOLVING

Southern Connecticut State University

Dr. Robert J. Snyder
Jennings 343 (203) 392-6263

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Text: *Introduction to Infrared and Raman Spectroscopy*, Third Edition, N. B. Colthrup, L. H. Daly, S. E. Wiberley, Academic Press (1990)

Introduction: Infrared Spectroscopy is the most powerful single technique available for the determination of molecular structure and the qualitative identification of unknown organic materials. Only an infrared spectrum yields direct information about the presence or absence of key functional groups. In addition, a match between the infrared spectrum of an unknown material and the spectrum of a reference sample is almost without equal as an empirical proof of identity.

Course Overview: The course will include a discussion of the theory of infrared spectroscopy, the differences between dispersive IR and Fourier-Transform IR, as well as Raman spectroscopy. Sample handling techniques, including solids, liquids, gases, and solutions will be covered in detail and the more modern ways of acquiring infrared data by reflectance will also be presented. Both internal (MIR and diffuse) reflectance and external (specular) reflectance techniques will be introduced. The students will be shown how to interpret infrared spectra using group frequencies, and how to process data using modern computerized techniques, such as smoothing and flattening, as well as the ability to take the difference between two spectra and the use of merging together two infrared spectra. And, if time allows, the course will conclude with a discussion of the most recent applications of IR, the combined techniques of GC/FT-IR and TGA/FT-IR. While not a laboratory course, the students will receive a liberal sampling of actual hands-on experience as well as classroom instruction.

Final Course Evaluation:

Mid-Term Examination	30%

Final Examination	30%
Course Project	40%

COURSE OUTLINE

Date	Topic
January 24	Spectroscopy-An Introduction
January 31	Theory of Vibrational Spectroscopy
February 7	Theory of Vibrational Spectroscopy
February 14	The Raman Effect-Fundamentals of Raman Spectroscopy
February 21	Infrared Instrumentation-Dispersive Spectrophotometers
February 28	Infrared Instrumentation-FT-IR Spectrometers
March 6	Infrared Instrumentation-FT-IR Spectrometers
March 13	**MID-TERM EXAMINATION**
March 20	Spring Break
March 27	Sampling Techniques for Infrared Analysis-Transmission Techniques
April 3	Sampling Techniques for Infrared Analysis-Transmission Techniques
April 10	Sampling Techniques for Infrared Analysis-Reflectance Techniques
April 17	Computer Methods in Infrared Analysis
April 24	Infrared Spectral Interpretation
May 1	Infrared Spectral Interpretation
May 8	Combined Analytical Techniques-GC/FT_IR and TGA/FT-IR
May 15	**FINAL EXAMINATION**

The exam questions will be taken directly from the material covered in class. The mid-term examination will be 1 1/2 hour long and there will be a one hour lecture following the exam. The final will be two hours long.

COURSE PROJECT: JOURNAL ARTICLE REVIEW

1. JOURNAL ARTICLE

Select an original research journal article from the 1995-1996 literature. The journal must be of the peer-reviewed type, such as *Analytical Chemistry, Applied Spectroscopy, Spectrochimica Acta Part B, or Journal of the American Chemical Society.* Articles from free, advertising-supported magazines such as *American Laboratory* and *Spectroscopy* are not allowed.

The article must be an original research paper, as opposed to a review article such as "A-page" articles in *Analytical Chemistry*. Unusually short articles and "Research Notes" are also not appropriate.

The article may cover a new technique, improvements in instrumentation or methods, or an application of a technique to a specific analysis (or any combination of these).

Approval for the article must be obtained from the course instructor. To obtain approval, bring a copy of at least the first page of the article to the instructor before or after class.

2. WRITTEN REVIEW OF ARTICLE

The review should be a minimum of 10 typewritten pages, but can include some figures or tables from the original article (or other articles) if they are appropriate to the review. A copy of the original article should also be included with the review.

While the exact format of the review is flexible, it should contain several key elements:

a) a review of the current status of the area of research (why was this work publishable?)
b) a synopsis of the paper, including experimental design, results, discussions, and conclusions
c) your critical evaluation of the paper, including answers to questions such as; is it a good paper? why or why not? are explanations too detailed or not detailed enough? what might have been done differently? is it understandable?is it appropriate?
d) your evaluation of the significance of the research (this is the most important part of the review as it involves a good understanding of the specific research topic and of infrared spectroscopy in general)

As always, the written work must be your own. Only a

minimum of direct quotes from any article are acceptable, and these must be clearly delineated and referenced. Grammar and spelling are important; poorly written articles will be penalized.

3. IMPORTANT DATES/DEADLINES FOR COURSE PROJECT

February 21	Deadline for approval of article to be reviewed
April 24	Review Article due (severe penalties for late projects)

I am well aware that most of you are part-time students with a full-time job and that your job may require that occasionally you have to miss a class. If you must travel or otherwise miss a class the week of the exams or when the journal article assignments are due, please let me know so that we can work something out.