Chemistry 3370a
Organic and Inorganic Structure Elucidation

A Notice from the Registrar:
"Unless you have either the prerequisites for this course or written special permission from your Dean to enroll in it, you will be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites."
Prerequisites: Either Chemistry 2273A and 2283G or Chemistry 2213A/B, either Chemistry 2271A and 2281G or Chemistry 2211A/B.

Instructor: Professor Brian L. Pagenkopf, Ph.D.

Class Times
Thursday, 8:30 – 10:30 KB K106
Friday 10:30-11:30, KB K106

Office Hours: by appointment, BGS 2020;
Thursday or Friday after class - time permitting

Course email: bpagenko@uwo.ca (start the subject line with 3370)

Text and web resources:

Introduction to Spectroscopy, 5th Edition, Pavia/Lampman/Kriz/Vyvyan

Note that there is little change within the chapters from the 4th edition so if you have access to one of those that might be an option, except that many of the homework problems have been changed. And the chapters have been reorganized.

Students should check OWL (http://owl.uwo.ca) on a regular basis for news and updates. This is the primary method by which course information will be disseminated to all students in the class. The missing of critical information due to your failure to check OWL cannot be used as a basis for appeal.

There are many spectroscopy websites, and these are particularly useful.

Spectroscopy overview:
http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/spectro.htm#contnt
A mathematical approach to NMR: http://www.cis.rit.edu/htbooks/nmr/inside.htm
Reich’s NMR site: http://www.chem.wisc.edu/areas/reich/chem605/index.htm
Course material

This course will rely heavily on the material in *Introduction to Spectroscopy*, 5th Edition by Pavia/Lampman/Kriz/Vyvyan

The text will be used extensively as the working class where the basic principles of each technique, trends, and how to extract structural information will be provided. It is also a source of numerous problems to integrate the ideas and provide practical experience. Note the useful appendices at the back of the book listing important values. Also note questions with an asterisk (*) have answers provided at the back of the text. Additional supplemental problems will also be provided from time to time. There are a lot of spectroscopy resources free on line (see above).

Topics to be covered will likely include:

**Molecular Formulas**: how they are obtained and information they provide. Elemental Analysis. Mostly self-study (Chapter 1)

**Mass Spectrometry**: Instrumentation, Ionization Methods, Interpretation of EI Mass Spectra for molecular weight, molecular formulas, fragmentation patterns for structural analysis. (Chapters 3 and 4)

**Infrared Spectroscopy**: Theory, Instrumentation, Characteristic Functional Group Absorptions, Analysis of a Spectrum (Chapter 2)

**Nuclear Magnetic Resonance Spectroscopy**: Basic concepts and review of simple proton and carbon NMR spectroscopy, NMR spectroscopy of other important I = ½ nuclei, relaxation and saturation, nuclear shielding, spin-spin coupling (homo and heteronuclear), first order spectra, equivalence and second order effects, effects of exchange and quadrupolar nuclei, correlation and 2D spectroscopy. (Chapters 5, 6, 7, 8 and 9)

**UV-visible Absorption Spectroscopy**: Brief introduction in its use (or lack of use) for structural elucidation (Chapter 10)
X-Ray Crystallography: Brief introduction and structural information it provides. (Optional supplemental material)

Learning Outcomes:

- Recognize the importance of spectroscopy in underpinning chemistry and importance for physical sciences.
- Think critically about, explain, integrate, and apply spectroscopic principles, laws, and theories.
- Solve structural problems using a variety of spectroscopic techniques.
- Diagram the basic hardware for instrumentation for UV/VIS, IR, mass spectroscopy and NMR.
- Become proficient and fast at interpreting routine 1H NMR spectra.
- Interpret routine spectra from a variety of techniques including IR, mass spectroscopy and NMR.
- Identify advantages and shortcomings in spectroscopic techniques.
- De-convolute complex first order NMR apparent multiplets into dd’s, ddd’s, dddd’s and ddddd’s.
- Use mass spectroscopy to distinguish between isomeric structures of identical mass.
- Solve complex structures or gain information from COSY, HSQC, HMBC, NOESY and INADEQUATE experiments.
- Draw basic pulse sequences for NMR experiments.
- Explain in qualitative terms the benefits of NMR experiments employing gradients.

Evaluation:

The final grade for the course will be determined by the following:

- Several assignments/quizzes 20%
- Term Test 30%
  
  Date: Wednesday November 11, 6:00 pm – 8:00 pm (3M 3250)

- Final Exam 50% (cumulative; 3 hours)
  
  Time and location set by Registrar

Failure to write the midterm test or final exam will result in a zero grade in the course, unless a valid excuse has been filed with the Dean's Office. It is the student's responsibility to ensure that medical notes for medical related absence or other acceptable documentation for other
reasons are filed with the Dean’s Office. Once notified by the Dean’ office the instructor will make the appropriate accommodation.

See: http://www.uwo.ca/univsec/handbook/appeals/accommodation_medical.pdf

IMPORTANT: If the midterm tests are missed for valid reasons, the final examination will be reweighted to include the weight of the missed midterm test. There are no alternate midterm tests. In case of a conflict see the instructor.

If a student’s performance on the final exam is better than on the term test the weighting of the two examinations may be altered to benefit the student at the instructor’s discretion. If used, the same reweighing opportunity will be applied to all students where beneficial.

The assignments/ quizzes

A few times throughout the term (sometimes every week, sometimes more spread out) there will be a short assignment based on recent lecture material or perhaps an announced or unannounced pop quiz.

Policy on Accommodation for Medical Illness

One missed assignment/quiz/activity for medical reasons will not require documentation, but two or more missed assignments/ quizzes/ activities will.

It is Faculty of Science policy that a student who chooses to write a test or exam deems themselves fit enough to do so, and the student must accept the mark obtained. Claims of medical, physical, or emotional distress after the fact will not be considered.

Statement on Use of Electronic Devices

No electronic devices are allowed during quizzes, tests or exams. It might be discussed in class if a specific model of a very basic calculator will be allowable.

Statement on Academic Offences

Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at this website: http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf.
Accessibility

Please contact the course instructor if you require material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 ext. 82147 if you have questions regarding accommodation.

Support Services

Learning-skills counsellors at the Student Development Centre (http://www.sdc.uwo.ca) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Students who are in emotional/mental distress should refer to Mental Health@Western (http://www.health.uwo.ca/mental_health) for a complete list of options about how to obtain help.

Additional student-run support services are offered by the USC, http://westernusc.ca/services. The website for Registrarial Services is http://www.registrar.uwo.ca.