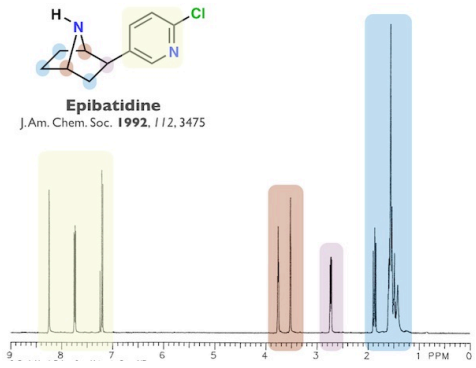

CHEMISTRY 754

Organic Spectroscopy Lab, Fall 2015

Instructor: Professor Gregory R. Cook
Office: Ladd 104G
Telephone: 231-7413
Email: Gregory.cook@ndsu.nodak.edu
Office Hours: by appointment
WEBPAGE: cook.chem.ndsu.nodak.edu

INTRODUCTION: The lab course is designed to train users on the various instruments for spectroscopic determination of organic compounds and to interpret data. Users will run known and unknown samples on the GC-Mass Spec, Infrared spectrometer, and NMR instruments. The knowledge gained from Chem 744 will aid in analyzing the data obtained.

GRADING: Grades will be assigned as follows: A 90-100%; B 80-89%; C 70-79%; D 60-69%; F <60%. Grades are based upon two laboratory reports; one for a known sample (40%) and one for an unknown sample (60%). In analyzing the data obtained, the following approximate percentages will be applied to the various spectroscopic techniques: Mass Spec - 20%, IR - 15%, NMR (^{1}H, ^{13}C, etc) - 65%.

PLAN: If you are not already trained, you should make arrangements with Dan Wanner or John Bagu to be trained on the NMR and IR, and Angel Ugrinov for training on the mass spectrometer. This should be done as soon as you can. Once trained, you will be provided with a known sample to analyze. You must obtain a MS, IR, ^{1}H NMR, and a ^{13}C NMR spectrum. In addition, 2D NMR (eg. COSY, HETCOR, NOESY) should be obtained to elucidate stereochemistry. An analysis of the spectral data (details below) should be written in a report to be due by Monday, October 19. When the report for your known sample is turned in, you will be given an unknown sample for structure determination. Again, you will need to obtain MS, IR, and NMR data (including 2D) for your sample. An analysis of the spectral data will be written in a report due by Monday, November 30. Late reports will incur a penalty of 10% per day.

REPORTS: You are expected to write a typewritten report in which you analyze all data obtained and relate it to the structure. The report should be written in manuscript style as if it were being submitted to a journal for publication. A good model to follow would be a paper on the structure determination of a natural product found in *J. Am. Chem. Soc.* All your data should be written as "experimental data" in ACS style at the end of your report (See *J. Am. Chem. Soc.* or *J. Org. Chem.*). Pertinent spectroscopic data which relates to the discussion of your structure should be put in tables or in the body of the text where appropriate. Your reports should include copies of all spectral data as an appendix.

MS - Determine the m/e peak and m+1 and m+2 if present. Explain the fragmentation patterns observed for as many peaks as possible. You should include the structure of the fragments as well as the fragmentation pathway from which it arose.
IR - Identify all functional groups in your molecule.
^{1}H NMR - Assign all resonances to the protons on the structure. All coupling constants should be calculated and splitting patterns explained.
^{13}C NMR - Assign all resonances to the carbons on the structure. Advanced NMR experiments may be necessary to correlate the peaks.
2D NMR - Explain your analysis of the data as it pertains to your structure.

Special Needs: Any students who need special accommodations for learning or who have special needs are invited to share these concerns or requests with the instructor as soon as possible.

Academic Responsibility: It is assumed that students at NDSU have the integrity to complete examinations on their own. I will provide an examination environment that discourages temptation otherwise. Any student who is found to have acted dishonestly on an exam will receive an F for the course. The policy applied is that of the Code of Academic Responsibility and Conduct as outlined in NDSU University Senate Policy, Section 335: Code of Academic Responsibility and Conduct (http://www.ndsu.nodak.edu/policy/335.htm).