

**Graduate Course in Spectroscopy/Small Molecule Structure Elucidation
(Fall 2008) -MacMillan**

This course is intended for all graduate students in need of the tools and techniques of modern structure elucidation, with the main focus of the course on NMR spectroscopy. The course will begin with an introduction to a variety of spectroscopic techniques (IR, UV, MS and NMR), cover the fundamental principles of NMR and spend considerable time teaching interpretation of data. We will also combine this course with a hands-on learning experience on the Varian instruments in the department.

Course Materials:

Primary Text:

“Spectroscopic Identification of Organic Compounds”, Silverstein, R. 7th Edition, Silverstein

Reference Material:

“Structure Determination of Organic Compounds: Tables of Spectral Data”, Pretsch, E.

Class Time: M, 9:00-10:30

Course Requirements:

Points:

Problem Solving / Participation	100
Unknown / Practical	100
Final	<u>150</u>
Total	450

Problem Solving: We will have problem solving sessions throughout the course (also during the Friday Advanced Problem Course). Each student will be responsible for leading one of the sessions.

Unknown: A goal of this course is to make everybody comfortable with hands on use of the Varian instruments, including tuning, shimming and acquiring complex experiments. Each student will be given 20 mg of an unknown compound for complete structural determination using NMR spectroscopy. More details will be provided later in the course. This will also give you an opportunity to learn the data processing software MestReNova.

Final: The final will be composed of theory and problem solving.

Course Schedule

<u>Date</u>	<u>Topic</u>
08/25	Intro / UV, IR
09/01	<i>Labor Day- no class</i>
09/08	UV, IR II
09/15	Mass Spec I (Jeff McDonald)
09/22	Mass Spec II (Jeff McDonald)
09/29	Intro to NMR - Theory
10/06	NMR Theory II
10/13	¹ H NMR - Chemical Shift, coupling
10/20	¹ H NMR - Chemical Shift, coupling
10/27	¹³ C NMR
11/03	2D NMR I
11/10	2D NMR II
11/17	Problem Solving
11/24	Other NMR Nuclei
12/01	Stereochemistry by NMR
12/08	Final Exam