

004:221

Spectroscopic Methods in Organic Chemistry

Spring, 2007

Instructor: Dr. Jim Gloer; Office, 531 CB; Phone, 335-1361; Email, james-gloer@uiowa.edu

Office Hours: 11:00-12:00 TTh; other meetings can be arranged by appointment.

Books: No specific textbook is *required* for the class, although two books are recommended as options to consider for useful reference materials. One is basically a compendium of data that provides many examples of spectral data for various types of compounds. This book is called *Structure Determination of Organic Compounds, Tables of Spectral Data*, and was authored by Pretsch, Buhlmann, and Affolter in 2000 (ISBN 3540678158). An earlier edition of this book would also be adequate. The second is a more traditional book (*Spectrometric Identification of Organic Compounds*, 7th edition, by Silverstein, Webster, and Kiemle, 2005, ISBN 0471393622). This edition is improved over its predecessors by virtue of the presence of more practice problems, as well as some updating of the content.

Efforts in this class will focus heavily on spectral interpretation, and this is best learned by covering basic principles and trends, looking at examples, and working problems. Because of this emphasis on practical applications, we will not have time to cover theoretical aspects of the various techniques in the depth that they deserve. We will cover relevant theory to some degree in the course notes (see below). However, you may wish to obtain a “traditional” text in this area that can serve as a helpful source of detailed, complementary explanations, as well as examples and practice problems beyond those to be provided in the course. There will be no specific assignments from either of these books, and that is why I do not require them, but students in the past who have commented about them have found them useful. Both books can be purchased online from various sources.

Other reasonable options aside from the one recommended above are available, *Organic Structure Analysis* (P. Crews, J. Rodriguez, and M. Jaspars), published in 1998, is one we have used in the past, but it has not been recently updated. Either this book or an older edition of the one above would serve as a good source of additional information, explanations, examples, illustrations, and problems. Copies of these and/or similar books will be placed on library reserve.

Course Notes: Copies of the course notes (i.e., the overheads used in class) will be provided as the semester progresses. Efforts will be made to make these available before class, so that students may add written comments to them during the lecture and, ideally, look them over before class. However, every year, some changes, deletions, and additions are typically made during the semester in an effort to keep the course updated and improve the quality of the notes, so the entire set cannot be made available at the beginning of the course.

Lectures: 9:30-10:45 AM TTh in room C29 PC. It may be necessary to cancel or reschedule one or two lectures during the semester due to schedule conflicts. If any class meetings need to be cancelled or rescheduled, advance notice will be given in class. Exams will be held outside of the regular class time, and this should give us some flexibility in making up any lost lecture periods. Because 75 min is a long time to sit and listen to a lecture, we have traditionally taken a 5 min break in the middle and extended the period to 10:50 AM, and I will plan to do the same this year. If anyone has any objection to this practice, please let me know.

Exams: There will be two exams and a final. Times, dates, and places for exams will be arranged in class to accommodate student schedules. Exams will be open-book and cumulative, and will consist mostly of spectral interpretation and related types of problem-solving. A sizeable block of time is generally needed for each exam, so they are usually held in the evenings.

Course Grades: Grades will be based on exam performance. The two mid-term exams will each be worth 30 percent of the final grade, while the final exam will be worth 40 percent. Problem sets will be assigned to provide practice in problem solving, but will not be graded. Answer keys will be placed on reserve on the chemistry library web site, and many of these problems will be discussed in class.

Student Rights and Responsibilities: For UI policies on academic misconduct, plagiarism and cheating, forgery, student complaints concerning faculty actions, and procedures for complaints, see the Student Academic Handbook: http://www.clas.uiowa.edu/students/academic_handbook/ix.shtml.

Special Needs: I need to hear from anyone who has a disability which may require some modification of seating, testing, or other class requirements so that appropriate arrangements may be made. Please contact me during office hours. The Student Disability Services office is located in 3101 Burge Hall (335-1462).

Course Content and Outline: This course will cover the most commonly used spectroscopic and spectrometric techniques in organic structure elucidation, with the exception of x-ray crystallography. The vast majority of course time will be spent on modern NMR (*ca.* 70%) and MS methods (*ca.* 20-25%), their practical applications, and interpretation of data generated using these techniques.

- I. NMR Spectroscopy
 - A. General principles
 - B. Proton NMR
 - C. Carbon-13 NMR
 - D. Other Nuclei
 - E. FT NMR pulse sequences and relevant 1D NMR experiments
 - F. 2D-NMR

- II. Mass Spectrometry (MS)
 - A. Electron Impact MS
 - B. Fragmentation
 - C. High Resolution MS
 - D. Soft-ionization techniques (ESI, FAB, CI, MALDI, etc.)
 - E. MS-MS and other experiments

- III. IR, UV, and CD Spectroscopy