Instructor: Prof. Jim Gloer; Office, E515 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 three books are recommended as options for you to consider as possible 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. The most recent (4th) edition of this book was published in 2009 and was authored by Pretsch, Bühlmann, and Badertscher (ISBN 3540938095). An earlier edition would also be adequate, e.g., the 2000 edition, authored by Pretsch, Bühlmann, and Affolter (ISBN 3540678158). The other two are more traditional books. Spectrometric Identification of Organic Compounds, 7th edition, by Silverstein, Webster, and Kiemle (2005, ISBN 0471393622) is improved over its predecessors by virtue of the presence of more practice problems, as well as some updating of the content. Another option is Organic Structure Analysis, 2nd Edition (P. Crews, J. Rodriguez, and M. Jaspars, ISBN 9780195336047; 2010). This is an improved edition of a book first published in 1998, and it is more detailed than the Silverstein book (though it is substantially more expensive). Either of these would serve as a good source of additional information, explanations, examples, illustrations, and problems. Of course, nowadays there are a lot of web resources one could also use. Links to some of these resources will be posted on the course ICON site.

Efforts in this class will focus heavily on spectral interpretation, and this is best learned by covering basic principles and trends, discussing 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, a “traditional” text in this area like those suggested above 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 assignments from any of these books, but students in the past who have commented about them have found them useful. These books can all be purchased online from various sources.

Course Notes: Copies of the course notes (i.e., the Powerpoint slides used in class) will be provided for download (in pdf format on ICON) as the semester progresses. These will be made available before they are covered in 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, clarify points, and improve the quality of the notes, so the entire set is not made available at the beginning of the course.

Lectures: 9:30-10:45 AM TTh in room E203 CB. It may be necessary to cancel or reschedule one or two lectures during the semester due to 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 minutes is a long time to sit and focus, we have traditionally taken a 5-minute break in the middle of the class and extended the period by 5 minutes. Unless someone has an objection to this
practice, I plan to do the same this year. Logistics for this will be discussed in class and will depend on student schedules (and on whether there is a class immediately after ours in the same room).

Once we get to a suitable point in the notes, we will often alternate between covering further notes and working through problems during class meetings in an effort to break things up. Students often view problem-solving in class as a particularly valuable element of the course content, so efforts will be made to dedicate as much of our class time to it as possible. Class participation will make this process more useful for everyone. Please do not be concerned about asking any question—all questions are welcome. Sometimes the simplest questions are the best...

**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 almost entirely of spectral interpretation and related types of problem-solving. A large block of time is generally needed for each exam, so they are usually held in the evenings. Exam I is typically held sometime during the week before Spring Break.

**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. Grades will be curved and assigned depending on the performance of this year's class on the exams.

Several problem sets will be assigned to provide practice in problem solving and exposure to different kinds of situations and data sets, but will not be graded. Answer keys will be posted on ICON, but most, if not all, of these problems will be discussed in class. In fact, efforts will be made to work most of them in class before the keys are posted so that they can be used to maximum effect in developing problem-solving skills and experience.

**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. 75%) and MS methods (ca. 20%), their practical applications, and interpretation of data generated using these techniques. Exam I will focus on interpretation of standard ¹H and ¹³C NMR data, while Exam II will build upon knowledge from Exam I by bringing in more sophisticated NMR techniques (including 2D NMR), and mass spectrometry. The Final Exam will be comprehensive, and will include problems of the same types found on Exams I and II, along with coverage of a few additional minor topics.

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I. **NMR Spectroscopy**
   A. General principles
   B. ¹H NMR
   C. ¹³C 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. **Selected Aspects of IR, UV, and CD Spectroscopy Relevant to Organic Chemistry**
Additional Information about Collegiate Policies and Procedures
The following policy and procedural statements have been summarized from the web pages of the College of Liberal Arts and Sciences and The University of Iowa Operations Manual.

Administrative Home. The College of Liberal Arts and Sciences (CLAS) is the administrative home of this course and governs matters such as the add/drop deadlines, the second-grade-only option, and other related issues. Different colleges may have different policies. Questions may be addressed to 120 Schaeffer Hall, or see the CLAS Student Academic Handbook.

Electronic Communication. University policy specifies that students are responsible for all official correspondence sent to their University of Iowa e-mail address (@uiowa.edu). Faculty and students should use this account for correspondence. (Operations Manual, III.15.2. Scroll down to k.11.)

Accommodations for Disabilities. A student seeking academic accommodations should first register with Student Disability Services and then meet privately with the course instructor to make particular arrangements. See www.uiowa.edu/~sds/ for more information. Their office is located in 3101 Burge Hall (335-1462).

Academic Honesty. Plagiarism and any other activities wherein students misrepresent work that is not their own, cheat on exams, etc. are considered academic fraud. Academic fraud is a serious matter and is reported to the departmental executive officer (DEO) and to the appropriate Associate Dean. Instructors and DEOs decide on appropriate consequences at the departmental level while the Associate Dean enforces additional consequences at the collegiate level. See the CLAS Academic Fraud section of the Student Academic Handbook.

CLAS Final Examination Policies. Final exams may be offered only during finals week. No exams of any kind are allowed during the last week of classes. The final examination schedule for each class will be announced around the fifth week of the semester by the Registrar. For this particular class in the past, we have successfully sought permission to extend the assigned period beyond the standard two hours by either adding a period before or after the assigned one, but otherwise, your instructor has no input into this schedule, and students should not ask their instructor to reschedule a final exam. Questions about this policy should be addressed to the CLAS Associate Dean for Undergraduate Programs and Curriculum.

Suggestions or Complaints. Students with a suggestion or complaint about this course should first visit the instructor, then the Departmental DEO. The Chemistry DEO can be contacted by calling the Chemistry Department front office at 335-0200. Complaints must be made within six months of the incident—see the CLAS Student Academic Handbook.

Understanding Sexual Harassment. Sexual harassment subverts the mission of the University and threatens the well-being of students, faculty, and staff. All members of the UI community have a responsibility to uphold this mission and to contribute to a safe environment that enhances learning. Incidents of sexual harassment should be reported immediately. See the UI Comprehensive Guide on Sexual Harassment for assistance, definitions, and the full University policy.

Public health authorities recommend that people with flu-like illnesses stay home and not return to public spaces until 24 hours after they have no fever. In order to prevent the spread of disease, please do not come to class, meet with other groups of students, attend office hours, or contact offices in person while you are ill with a fever.

Reacting Safely to Severe Weather. In severe weather, class members should seek appropriate shelter immediately, leaving the classroom if necessary. The class will continue if possible when the event is over. For more information on Hawk Alert and the siren warning system, visit the Public Safety web site.