C. Eugene Bennett Department of Chemistry  
West Virginia University  
Graduate Program  

Chemistry 793C  
Special Topics: Organic Structure Characterization Syllabus  

**COURSE INFORMATION:**  
Semester, Year: Spring 2012  
Meeting day, time: Monday/Wednesday/Friday, 09:30 – 10:20 am  
Meeting Location: 260 Hodges Hall  

**COURSE WEBPAGE:**  
http://community.wvu.edu/~bvp003/1/Courses.html  

- A Dropbox site will also be made available for sharing of electronic documents  

**CONTACT INFORMATION:**  
Instructor: Dr. Brian Popp, Assistant Professor  
Office: CRL 457  
Lecture Preparation: Monday/Wednesday/Friday 8:00 – 9:20 am  
Office Hours: Open-Door and By Appointment  
Email: Brian.Popp@mail.wvu.edu  
Phone: 304-293-3435 ext. 6447  

**COURSE OVERVIEW:**  
This course will provide a general foundation for identifying the functionalities and elucidating the bond connectivity of unknown organic molecules using NMR and IR spectroscopy and mass spectrometry techniques. A significant percentage of the course will be dedicated to the interpretation of one- and two-dimensional NMR spectra based on observed chemical shift, through-space and through-bond coupling, and relaxation processes.  

**EXPECTED LEARNING OUTCOMES:**  
Upon successful completion of this course, the student will be able to:  
1) Recognize the importance of spectroscopic and spectrometric techniques in chemical synthesis.  
2) Understand the fundamental magnetic properties of certain nuclei that lead to signals in NMR spectroscopic experiments  
3) Appreciate basic aspects of NMR experiments (pulse sequences) that yield specific chemical or structural data.  
4) Apply appropriate NMR experiments and interpretative strategies discussed in the course to assign correctly the structure of unknown compounds in their own research area.  

**PREREQUISITES:**  
This course is directed toward graduate students that have completed a one-year course in organic chemistry. Please see me outside of class if you have ongoing concerns about your background during the semester.


**Course Materials and Textbooks:**

This course will rely heavily on lecture materials from Prof. Hans Reich’s CHM 605: Structure Determination using Spectroscopic Methods at the University of Wisconsin-Madison. Electronic reference and lecture materials are available at:

HTTP://WWW.CHEM.WISC.EDU/AREAS/REICH/CHEM605/INDEX.HTM

  Students are required to purchase this textbook, as it will serve as a useful reference for their future research.

  Students are not required to purchase these texts; however, they may serve as a useful resource for future research. Table of data relevant to structure elucidation will be distributed during the course of the class.


My lectures may be supplemented with material from these texts—all of which are available in my office to borrow/copy on a limited basis. Many of these texts are excellent resources for more advanced applications of NMR spectroscopy.


**Problem Sets:** You will receive approximately one problem set per week at Friday’s class. These problem sets are due on at the beginning of class on the following Wednesday. Work will not be accepted late without a justified excuse. The problem sets are each worth 10 pts and will not be graded for correctness; rather, the problems will be evaluated to ensure that the student has attempted all problems with some sign of effort. Failure to attempt all problems will result in only 5 pts awarded. Problems will be reviewed with audience participation during the following Friday’s lecture.

**Take-Home Quizzes:** A periodic take-home quiz will be distributed. These quizzes will test relevant course content from lecture, reading, and homework assignments. These quizzes are the product of your own effort – no individual inside or outside of this course/department may contribute to your answers. You may however utilize all course notes, handouts, texts, Internet resources, etc. You will be asked to sign the front of the quiz verifying that you neither accepted nor provided answers to/from others on the quiz.

**Exams:** Three exams will cover materials in lectures, assigned readings, and problem sets in the first, middle, last segments of the semester, respectively. Although the Exams will not be comprehensive per say, material covered during the first segment of the course will likely prove important. The exams will be administered on either Tuesday or Wednesday evening from 6–8 PM – specific dates will be decided during the course of the semester. All lecture materials (including handouts, texts, lecture notes) may be used on the examination; no computers/electronic devices, with the exception of a calculator, will be permitted. Each individual must bring their own materials – there will be no sharing of materials during the examination.

**Course Outline and Reading Assignments (Tentative Ordering):**

- **Introduction to Spectroscopic Methods**  
  *(Reading Assignment: Simpson Chap. 1)*  
  *(Suggested Reading: Simpson Chap. 2-3)*

- **\(^1\)H NMR and \(^{13}\)C NMR Spectroscopy: The Basics**  
  *(Reading Assignment: Simpson Chap. 4-5)*

- **Combining Spectral Data for Structure Elucidation**  
  *(Reading Assignment: Simpson Chap. 9.1-9.6, 9.9, and Chap 10)*

- **\(^1\)H-\(^2\)H J Coupling Constants**  
  *(Reading Assignment: Simpson Chap. 6)*

- **\(^1\)H Chemical Shifts: Advanced Topics**

- **\(^{13}\)C J Coupling Constants**

- **Relaxation Processes**  
  *(Reading Assignment: Simpson Chap. 7 and 8.1)*

- **Dynamic NMR Spectroscopy**  
  *(Reading Assignment: Simpson Chap. 8)*

- **Homonuclear Two-Dimensional NMR Spectroscopy**  
  *(Reading Assignment: Simpson Chap. 9.7-9.8 and 9.10-9.11)*

- **Heteronuclear Two-Dimensional NMR Spectroscopy**

- **Other Nuclei (Spin ½ and Quadrupoles)**

- **Mass Spectrometry: Advanced Topics – Pending Availability of Time**
**Grade Breakdown:**

PROBLEM SETS (100 pts)  
10% FINAL GRADE  
TAKE-HOME QUIZZES (100 pts)  
10% FINAL GRADE  
IN-CLASS PARTICIPATION (100 pts)  
5% FINAL GRADE  

EXAM ONE (150 pts) – TBA – 6-8 PM  
25% FINAL GRADE  
EXAM TWO (150 pts) – TBA – 6-8 PM  
25% FINAL GRADE  
EXAM THREE (150 pts) – TBA – 6-8 PM  
25% FINAL GRADE

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<thead>
<tr>
<th>LETTER GRADE</th>
<th>GRADE POINT</th>
<th>GRADE RANGE</th>
<th>DESCRIPTION OF LEARNING OUTCOME</th>
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<tr>
<td>A</td>
<td>4.0</td>
<td>90-100</td>
<td>SUPERIOR ACHIEVEMENT</td>
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I reserve the right to reduce the lower limit of the grade range.

**Attendance and Participation:** I cannot stress enough how important class attendance is. If a student misses a class, he or she should get the notes from a fellow student. I strongly encourage the student to cover the missed material by scheduling a meeting time with me. Assignments that are not submitted on time due to unexcused absences will not be accepted late and will result in zero credit awarded.

**Scientific and Professional Ethics:**  
The integrity of the classes offered by any academic institution solidifies the foundation of its mission and cannot be sacrificed to expediency, ignorance, or blatant fraud. Therefore, I will enforce rigorous standards of academic integrity in all aspects and assignments of this course. For the detailed policy of West Virginia University regarding the definitions of acts considered to fall under academic dishonesty and possible ensuing sanctions, please see the Student Conduct Code [http://studentlife.wvu.edu/office_of_student_conduct/student_conduct_code](http://studentlife.wvu.edu/office_of_student_conduct/student_conduct_code). Should you have any questions about possibly improper research citations or references, or any other activity that may be interpreted as an attempt at academic dishonesty, please see me before the assignment is due to discuss the matter.

**Disability Accommodation:** If you require, or believe you require, disability accommodation, contact the Office of Disability Services (G30 Mountainlair, 3-6700). The Office will initiate the appropriate procedures/arrangements.