Chemistry 430, Structural Analysis of Organic Molecules  
Spring 2012

Course Times: Monday, Wednesday, and Friday, 11:15 a.m. – 12:05 p.m.
Course Location: 101 Osmond

Lecturer:
Dr. Kate Masters
Office: 218 Whitmore Lab
Phone: 863-3319
E-mail: kmasters@psu.edu
Office Hours: By appointment

Website: ANGEL, Chem 430, Section 001 Sp12


Course Content

This course is designed to teach you how to interpret spectral data for the purpose of elucidating structures of organic molecules. Some theoretical background will be given for various spectroscopic/identification methods, but the emphasis will be placed on solving problems, that is, interpreting and annotating the spectral data for pure compounds and for mixtures/impure compounds. Essentially, the goal is to give you an idea of what a synthetic organic chemist faces when analyzing compounds. Thus, this course will be taught from a very practical standpoint. Identification methods to be covered include UV/Vis spectroscopy, IR spectroscopy, mass spectrometry, and NMR spectroscopy.

Course Topics, in order of presentation:

1. UV/Vis Spectroscopy (Chapter 7, Pavia text)
2. Infrared Spectroscopy (IR) (Chapter 2)
3. Mass Spectrometry (MS) (Chapter 8)
4. 1D Nuclear Magnetic Resonance (NMR) (Chapters 3-6)
5. 2D NMR (Chapter 10)

For each of these topics, you encouraged to read the appropriate chapters indicated above. At the end of these chapters you will find *starred* problems. These problems’ answers are given near the end of the book, in the “ANS-1” section. You are encouraged to answer as many of these problems for practice; try to refrain from looking at the answer until you are satisfied with your answer.

In Pavia’s text, you will also find relevant and useful appendices, which may be useful for interpretation of data. The information in these appendices may or may not be given in the lecture notes; be aware that they are in the textbook, and you can use them during group questions and final exams.
Practice Problems

In addition to the problems found in Pavia’s text, the following websites contain practice spectral problems:

WebSpectra: http://www.chem.ucla.edu/~webspectra/
Organic Structure Elucidation: http://www.nd.edu/~smithgrp/structure/workbook.html
Organic Spectral Analysis Problems: http://home.millsaps.edu/kramewh/Fertig/startspecpage.html

Grades

Earned points are accumulated by the following: group questions (weighted to equal 20% of the final grade), six homework sets (in total, weighted to equal 15% of final grade), three mid-semester cumulative exams (in total, weighted to equal 45% of final grade; each exam is weighted to equal 15% of the final grade), and a comprehensive, final exam (weighted to equal 20% of the final grade). The typical overall average in this course is a grade of B. Class participation is important and will be considered in cases where a student is close to a grade cutoff.

Group Questions (20% of Final Grade)

The purpose of group questions is to get students to participate in the class and for the instructor to get frequent feedback on student understanding of concepts. Groups of three or four students will form by the end of the second week of the semester. Questions will be given out, discussed, and collected during lecture. The questions will be worth varying points; they (in total) are weighted to equal 20% of the final grade. Each group member present will get one shared grade for these questions, thus it is important that everyone in the group participates equally and shows up for lecture! The lowest three (3) grades (in %) for each individual person will be dropped.

Homework Sets: Textbook Problems (15% of Final Grade)

Six homework sets will be assigned throughout the semester and will be problems taken from Pavia’s textbook (given below). All combined homework sets will be weighted to equal 15% of the final grade. Due dates will be given in lecture. For each answer, you are required to give your rationale for your answer. You are welcome to photocopy the problem and write out your rationale or to sketch spectra with your explanation.

- Homework Set 1 on UV/Vis: Chapter 7, Questions 7 and 8 (a) & (b)
- Homework Set 2 on IR: Chapter 2, Questions 8, 9, and 10
- Homework Set 3 on 1D $^1$H & $^{13}$C NMR: Chapter 3, Questions 25 and 27; Chapter 4, Questions 11 and 13
- Homework Set 4 on Proton Coupling in $^1$H NMR: Chapter 5, Questions 9, 11, and 20
- Homework Set 5 on Combined Problems: Chapter 9, Questions 19, 21, 25, and 33
- Homework Set 6 on 2D NMR: Chapter 10, Questions 2 and 8
Exams (65% of Final Grade): Three Mid-Semester Exams (each 15% of final grade); a final exam (20% of final grade)

All exams will be take-home; the honor system will be implemented to ensure that you work by yourself and without the use of online databases/libraries or textbook solution manuals. The exams will mainly include short-answer questions. They will be constructed in such a way as to emphasize active understanding of the material. All exams are cumulative.

All exams will be handed out during Monday’s lecture and will be due the next day (Tuesday). You will be required to “sign out” the exam. Your signature will indicate that you have read and understand the honor system policy. If you do not honor this system, you will receive a zero on the exam as the first offense. The second offense is a final grade of F or XF.

The mid-semester exam due date schedule is as follows:

- Exam 1: Tuesday, February 7 by 2:00 pm in 218 Whitmore
- Exam 2: Tuesday, March 13 by 2:00 pm in 218 Whitmore
- Exam 3: Tuesday, April 10 by 2:00 pm in 218 Whitmore
- Final Exam: During Finals Week, Day TBD

Exam Regrade Policy

Graded exams are handed back so that students can (a) see what kinds of mistakes they made and thus better prepare for future exams, and (b) determine if serious errors were made in grading, adding up points, etc. The purpose of regrading a question on an exam is not specifically to raise a student’s grade, although sometimes that may be the result. Instead, the purpose is to be certain that, within reason, the same grading standards were applied to all exams.

Grade lines must be drawn somewhere. It is unfortunate but inevitable that some students will miss a grade by only a few points, sometimes even just one point. It is the policy in this course to give partial credit for answers that are not completely correct but that have significant merit. By comparison to grading simply right or wrong, assigning partial credit is less precise.

With these considerations in mind, the following regrade policy will apply:

Regrade requests must be submitted in writing within three school days of the exam being returned. A regrade request must include: (1) the exam, (2) the answer key’s answer, copied on a separate piece of paper, and (3) an explanation in writing of why your answer deserves more credit.

If your request involves an arithmetic error in calculating your score, don’t bother with (2). Failure to follow these directions will automatically result in regrade requests being returned without any consideration.

Requests must be submitted within three lectures of the day the graded exam is handed back.
Procedures

Registrar Dates

Drop Period: Ends January 18, 2012
Add Period: Ends January 19, 2012 at 8 am
Late Drop Deadline: Ends April 6, 2012

Academic Integrity: Instructors are now asked (Senate Rule 49-20) to provide at the beginning of a course a statement to "clarify the application of academic integrity criteria to that course". The Senate Rule includes the following:

Academic dishonesty includes, but is not limited to, cheating, plagiarizing, fabrication of information or citations, facilitating acts of academic dishonesty by others, having unauthorized possession of examinations, submitting work of another person or work previously used without informing the instructor, or tampering with the academic work of other students.

(You should also be aware of the extensive parts of this Rule that describe procedures for handling alleged instances of academic dishonesty.) Specific instances of academic dishonesty in this course would include (but not limited to) copying or helping someone else copy during an examination, using unauthorized materials during an examination, stealing or destroying course materials or another student's examination paper, altering answers or grades on graded examinations, having someone take an examination for you, and attempting to do any of the above. Such infractions are considered cause, at the least, for awarding a grade of "0" on the exam in question (and not allowing the student to drop the class).
## Tentative Course Schedule, Spring 2012

<table>
<thead>
<tr>
<th>Week</th>
<th>Monday</th>
<th>Wednesday</th>
<th>Friday</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9-Jan</td>
<td>11-Jan</td>
<td>13-Jan</td>
</tr>
<tr>
<td></td>
<td>Course Overview</td>
<td>UV/Vis Spectroscopy</td>
<td>UV/Vis Spectroscopy</td>
</tr>
<tr>
<td>2</td>
<td>16-Jan No Class</td>
<td>18-Jan InfraRed Spectroscopy;</td>
<td>20-Jan InfraRed Spectroscopy</td>
</tr>
<tr>
<td></td>
<td>Martin Luther King, Jr. Day</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>30-Jan Mass Spectrometry</td>
<td>1-Feb Mass Spectrometry</td>
<td>3-Feb Mass Spectrometry</td>
</tr>
<tr>
<td>5</td>
<td>6-Feb Mass Spectrometry;</td>
<td>8-Feb Mass Spectrometry</td>
<td>10-Feb Mass Spectrometry</td>
</tr>
<tr>
<td></td>
<td><strong>Get Exam 1</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>13-Feb Mass Spectrometry</td>
<td>15-Feb Mass Spectrometry</td>
<td>17-Feb Mass Spectrometry</td>
</tr>
<tr>
<td>7</td>
<td>20-Feb Mass Spectrometry</td>
<td>22-Feb Mass Spectrometry</td>
<td>24-Feb 1D NMR</td>
</tr>
<tr>
<td>8</td>
<td>27-Feb 1D NMR;</td>
<td>29-Feb 1D NMR</td>
<td>2-Mar 1D NMR</td>
</tr>
<tr>
<td>9</td>
<td>5-Mar Spring Break</td>
<td>7-Mar Spring Break</td>
<td>9-Mar Spring Break</td>
</tr>
</tbody>
</table>

---

5
<table>
<thead>
<tr>
<th>10</th>
<th>12-Mar 1D NMR; <strong>Get Exam 2</strong></th>
<th>14-Mar 1D NMR</th>
<th>16-Mar 1D NMR</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>19-Mar 1D NMR</td>
<td>21-Mar 1D NMR</td>
<td>23-Mar 1D NMR</td>
</tr>
<tr>
<td>12</td>
<td>26-Mar 1D NMR</td>
<td>28-Mar 1D NMR</td>
<td>30-Mar 1D NMR</td>
</tr>
<tr>
<td>13</td>
<td>2-Apr 2D NMR</td>
<td>4-Apr 2D NMR</td>
<td>6-Apr 2D NMR</td>
</tr>
<tr>
<td>14</td>
<td>9-Apr 2D NMR; <strong>Get Exam 3</strong></td>
<td>11-Apr 2D NMR</td>
<td>13-Apr 2D NMR</td>
</tr>
<tr>
<td>15</td>
<td>16-Apr 2D NMR</td>
<td>18-Apr 2D NMR</td>
<td>20-Apr 2D NMR</td>
</tr>
<tr>
<td>16</td>
<td>23-Apr 2D NMR</td>
<td>25-Apr 2D NMR</td>
<td>27-Apr 2D NMR</td>
</tr>
<tr>
<td>17</td>
<td>Final Exam</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>